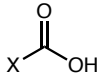
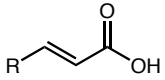
## INORGANIC ACIDS

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $H_2O$ | 15.7 | (32) |
| $H_3O^+$ | -1.7 | |
| $H_2S$ | 7.00 | |
| HBr | -9.00 | (0.9) |
| HCl | -8.0 | (1.8) |
| HF | 3.17 | (15) |
| HOCl | 7.5 | |
| $HClO_4$ | -10 | |
| HCN | 9.4 | (12.9) |
| $HN_3$ | 4.72 | (7.9) |
| HSCN | 4.00 | |
| $H_2SO_3$ | 1.9, 7.21 | |
| $H_2SO_4$ | -3.0, 1.99 | |
| $H_3PO_4$ | 2.12, 7.21, 12.32 | |
| $HNO_3$ | -1.3 | |
| $HNO_2$ | 3.29 | |
| $H_2CrO_4$ | -0.98, 6.50 | |
| $CH_3SO_3H$ | -2.6 | (1.6) |
| $CF_3SO_3H$ | -14 | (0.3) |
| $NH_4Cl$ | 9.24 | |
| $B(OH)_3$ | 9.23 | |
| HOOH | 11.6 | |

## CARBOXYLIC ACIDS



| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| X= $CH_3$ | 4.76 | (12.3) |
| $CH_2NO_2$ | 1.68 | |
| $CH_2F$ | 2.66 | |
| $CH_2Cl$ | 2.86 | |
| $CH_2Br$ | 2.86 | |
| $CH_2I$ | 3.12 | |
| $CHCl_2$ | 1.29 | |
| $CCl_3$ | 0.65 | |
| $CF_3$ | -0.25 | |
| H | 3.77 | |
| HO | 3.6, 10.3 | |
| $C_6H_5$ | 4.2 | (11.1) |
| *o*-$O_2NC_6H_4$ | 2.17 | |
| *m*-$O_2NC_6H_4$ | 2.45 | |
| *p*-$O_2NC_6H_4$ | 3.44 | |
| *o*-$ClC_6H_4$ | 2.94 | |
| *m*-$ClC_6H_4$ | 3.83 | |
| *p*-$ClC_6H_4$ | 3.99 | |
| *o*-$(CH_3)_3N^+C_6H_4$ | 1.37 | |
| *p*-$(CH_3)_3N^+C_6H_4$ | 3.43 | |
| *p*-$OMeC_6H_4$ | 4.47 | |

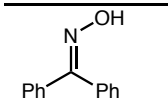


| | | |
|---|---|---|
| R= H | 4.25 | |
| *trans*-$CO_2H$ | 3.02, 4.38 | |
| *cis*-$CO_2H$ | 1.92, 6.23 | |

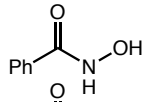
## ALCOHOLS

| | | |
|---|---|---|
| HOH | 15.7 | (31.2) |
| MeOH | 15.5 | (27.9) |
| *i*-PrOH | 16.5 | (29.3) |
| *t*-BuOH | 17.0 | (29.4) |
| *c*-$hex_3COH$ | 24.0 | |
| $CF_3CH_2OH$ | 12.5 | (23.5) |
| $(CF_3)_2CHOH$ | 9.3 | (18.2) |
| $C_6H_5OH$ | 9.95 | (18.0) |
| *m*-$O_2NC_6H_4OH$ | 8.4 | |
| *p*-$O_2NC_6H_4OH$ | 7.1 | (10.8) |
| *p*-$OMeC_6H_4OH$ | 10.2 | (19.1) |
| 2-napthol | | (17.1) |

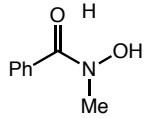
## OXIMES & HYDROXAMIC ACIDS



| | |
|---|---|
| 11.3 | (20.1) |



| | |
|---|---|
| 8.88 (NH) | (13.7) |

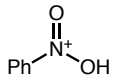


| | |
|---|---|
| | (18.5) |

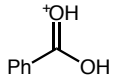
## PEROXIDES

| | |
|---|---|
| MeOOH | 11.5 |
| $CH_3CO_3H$ | 8.2 |

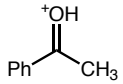
## PROTONATED SPECIES



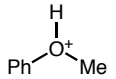
| |
|---|
| -12.4 |



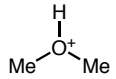
| |
|---|
| -7.8 |



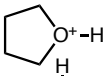
| |
|---|
| -6.2 |



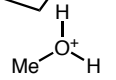
| |
|---|
| -6.5 |



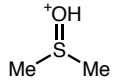
| |
|---|
| -3.8 |



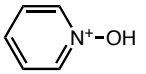
| |
|---|
| -2.05 |



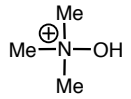
| |
|---|
| -2.2 |



| |
|---|
| -1.8 |

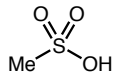


| | |
|---|---|
| 0.79 | (+1.63) |

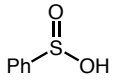


| | |
|---|---|
| | (+5.55) |

## SULFINIC & SULFONIC ACIDS



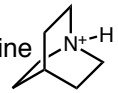
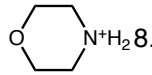
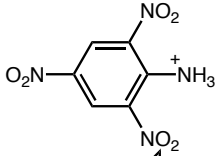
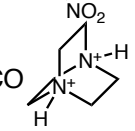
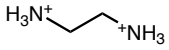
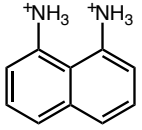
| |
|---|
| -2.6 |

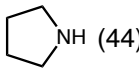
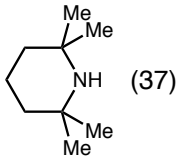
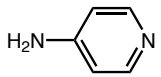
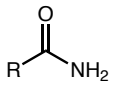
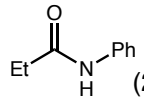
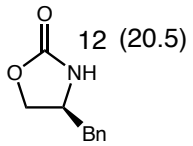
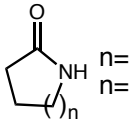
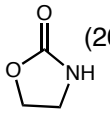
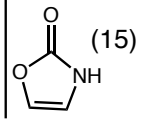
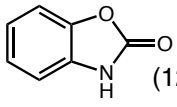


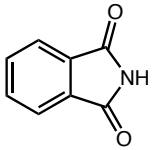
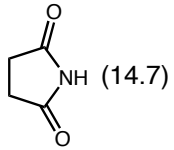
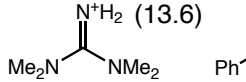
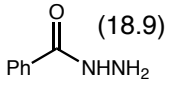
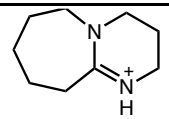
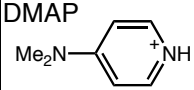
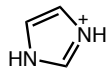
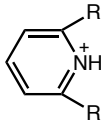
| |
|---|
| 2.1 |

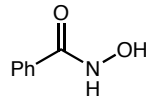
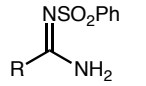
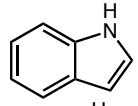
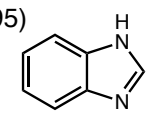
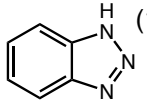
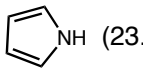
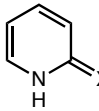
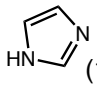
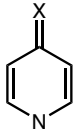
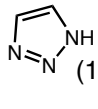
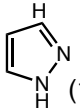
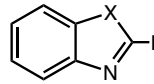
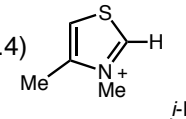
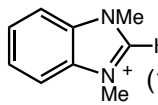
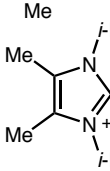
*Values <0 for $H_2O$ and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **PROTONATED NITROGEN** | | |
| $N^+H_4$ | 9.2 | (10.5) |
| $EtN^+H_3$ | 10.6 | |
| *i*-$Pr_2N^+H_2$ | 11.05 | |
| $Et_3N^+H$ | 10.75 | (9.00) |
| $PhN^+H_3$ | 4.6 | (3.6) |
| $PhN^+(Me)_2H$ | 5.20 | (2.50) |
| $Ph_2N^+H_2$ | 0.78 | |
| 2-napthal-$N^+H_3$ | 4.16 | |
| $H_2NN^+H_3$ | 8.12 | |
| $HON^+H_3$ | 5.96 | |
| Quinuclidine  | 11.0 | (9.80) |
| Morpholine  | 8.36 | |
| N-Me morpholine | 7.38 | |
|  | -9.3 | |
| DABCO  | 2.97, 8.82 (2.97, 8.93) | |
|  | 6.90, 9.95 | |
| Proton Sponge  | -9.0, 12.0 (--, 7.50) | |
| $PhCN^+H$ | -10 | |

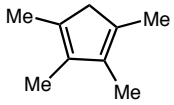
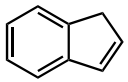
| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **AMINES** | | |
| $HN_3$ | 4.7 | (7.9) |
| $NH_3$ | 38 | (41) |
| *i*-$Pr_2NH$ | (36 THF)) | |
| $TMS_2NH$ | 26(THF) | (30) |
| $PhNH_2$ (30.6) | | |
| $Ph_2NH$ (25.0) | | |
| $NCNH_2$ (16.9) | | |
|  | (44) | |
|  | (37) | |
|  | (26.5) | |
| **AMIDES & CARBAMATES** | | |
|  | R= H | (23.5) |
| | $CH_3$ 15.1 | (25.5) |
| | Ph | (23.3) |
| | $CF_3$ | (17.2) |
| | (urea) $NH_2$ | (26.9) |
| | OEt | (24.8) |
|  | (21.6) | |
|  | 12 (20.5) | |
|  | n= 1 (24.1) n= 2 (26.4) | |
|  | (20.8) | |
|  | (15) | |
|  | (12.1) | |

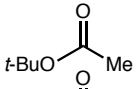
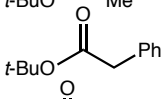
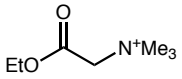
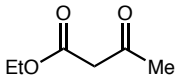
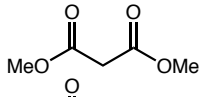
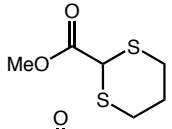
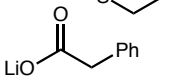
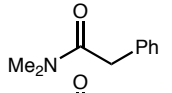
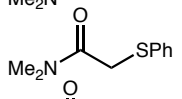
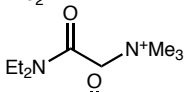
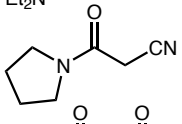
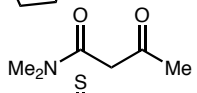
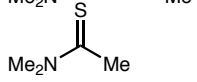
| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **IMIDES** | | |
|  | 8.30 | |
|  | | (14.7) |
| $Ac_2NH$ | | (17.9) |
| **SULFONAMIDE** | | |
| $RSO_2NH_2$ | R = Me | (17.5) |
| | Ph | (16.1) |
| | $CF_3$ 6.3 | (9.7) |
| $MeSO_2NHPh$ | | (12.9) |
| **GUANIDINIUM, HYRDAZONES,- IDES, & -INES** | | |
|  | $N^+H_2$ (13.6) | $NNH_2$ (21.6) |
|  | (18.9) | |
| $PhSO_2NHNH_2$ | | (17.2) |
| PhNHNHPh | | (26.1) |
| **PROTONATED HETEROCYCLES** | | |
| DBU  | (12) (estimate) | |
| DMAP  | 9.2  | 6.95 |
|  | R= H (PPTS) | 5.21 (3.4) |
| | *t*-Bu | 4.95 (0.90) |
| | Me | 6.75 (4.46) |
| | Cl, H | 0.72 |

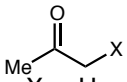
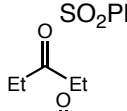
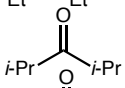
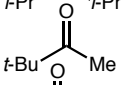
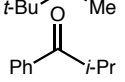
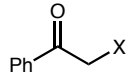
| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **HYDROXAMIC ACID & AMIDINES** | | |
|  | 8.88 (NH) | (13.7) |
|  | R= Me | (17.3) |
| | Ph | (15.0) |
| **HETEROCYCLES** | | |
|  | (20.95) | |
|  | (16.4) | |
|  | (11.9) | |
|  | (23.0) | |
|  | X= O (24) X= S (13.3) | |
|  | (18.6) | |
|  | X= O (14.8) X= S (11.8) | |
|  | (13.9) | |
|  | (19.8) | |
|  | X= O (24.4) X= S (27.0) | |
|  | (29.4) | |
|  | (16.5) | |
|  | (18.4) | |
|  | (24) | |

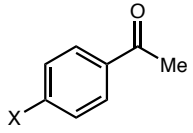
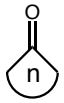
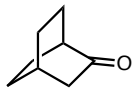
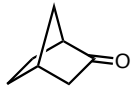
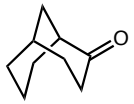
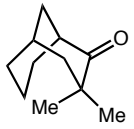
*Values <0 for $H_2O$ and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **HYDROCARBONS** | | |
| $(Me)_3CH$ | 53 | |
| $(Me)_2CH_2$ | 51 | |
| $CH_2=CH_2$ | 50 | |
| $CH_4$ | 48 | (56) |
| △ | 46 | |
| $CH_2=CHCH_3$ | 43 | (44) |
| PhH | 43 | |
| $PhCH_3$ | 41 | (43) |
| $Ph_2CH_2$ | 33.5 | (32.2) |
| $Ph_3CH$ | 31.5 | (30.6) |
| HCCH | 24 | |
| PhCCH | 23 | (28.8) |
| $XC_6H_4CH_3$ | | |
| X= *p*-CN | | (30.8) |
| *p*-$NO_2$ | | (20.4) |
| *p*-COPh | | (26.9) |
|  | | (26.1) |
|  | 20 | (20.1) |
|  | 15 | (18.0) |
| $H_2$ | ~36 | |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **ESTERS** | | |
|  | 24.5 | (30.3) |
|  | | (23.6) |
|  | | (20.0) |
|  | 11 | (14.2) |
|  | 13 | (15.7) |
|  | | (20.9) |
|  | | [30.2 (THF)] |
| **AMIDES** | | |
|  | | (26.6) |
|  | | (25.9) |
|  | | (24.9) |
|  | | (17.2) |
|  | | (18.2) |
|  | | (25.7) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **KETONES** | | |
|  | | |
| X= H | | (26.5) |
| Ph | | (19.8) |
| SPh | | (18.7) |
| $COCH_3$ | 9 | (13.3) |
| $SO_2Ph$ | | (12.5) |
|  | 19-20 | (27.1) |
|  | | (28.3) |
|  | | (27.7) |
|  | | (26.3) |
|  | | |
| X= H | | (24.7) |
| $CH_3$ | | (24.4) |
| Ph | | (17.7) |
| $COCH_3$ | | (14.2) |
| COPh | | (13.3) |
| CN | | (10.2) |
| F | | (21.6) |
| OMe | | (22.85) |
| OPh | | (21.1) |
| SPh | | (16.9) |
| SePh | | (18.6) |
| $NPh_2$ | | (20.3) |
| $N^+Me_3$ | | (14.6) |
| $NO_2$ | | (7.7) |
| $SO_2Ph$ | | (11.4) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
|  | | |
| X= H | | (24.7) |
| OMe | | (25.7) |
| $NMe_2$ | | (27.5) |
| Br | | (23.8) |
| CN | | (22.0) |
|  | | |
| n= 4 | | (25.1) |
| 5 | | (25.8) |
| 6 | | (26.4) |
| 7 | | (27.7) |
| 8 | | (27.4) |
|  | | (28.1) |
|  | | (29.0) |
|  | | (25.5) |
|  | | (32.4) |

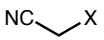
*Values <0 for $H_2O$ and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

# pKa's of CH bonds at Nitrile, Heteroaromatic, and Sulfur Substituted Carbon

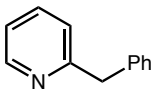
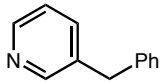
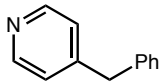
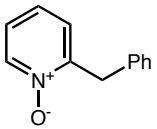
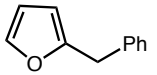
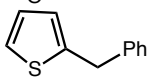


## NITRILES



| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | H | | (31.3) |
| | $CH_3$ | | (32.5) |
| | Ph | | (21.9) |
| | COPh | | (10.2) |
| | $CONR_2$ | | (17.1) |
| | $CO_2Et$ | | (13.1) |
| | CN | 11 | (11.1) |
| | OPh | | (28.1) |
| | $N^+Me_3$ | | (20.6) |
| | SPh | | (20.8) |
| | $SO_2Ph$ | | (12.0) |

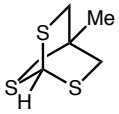
## HETERO-AROMATICS

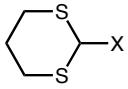
| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
|  | | (28.2) |
|  | | (30.1) |
|  | | (26.7) |
|  | | (25.2) |
|  | | (30.2) |
|  | | (30.0) |

## SULFIDES

$PhSCH_2X$

| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | Ph | | (30.8) |
| | CN | | (20.8) |
| | $COCH_3$ | | (18.7) |
| | COPh | | (16.9) |
| | $NO_2$ | | (11.8) |
| | SPh | | (30.8) |
| | $SO_2Ph$ | | (20.5) |
| | $SO_2CF_3$ | | (11.0) |
| | $POPh_2$ | | (24.9) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $MeSCH_2SO_2Ph$ | | (23.4) |
| $PhSCHPh_2$ | | (26.7) |
| $(PhS)_3CH$ | | (22.8) |
| $(PrS)_3CH$ | | (31.3) |
|  | | (30.5) |
| $(PhS)_2CHPh$ | | (23.0) |



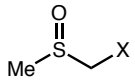
| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | Ph | | (30.7) |
| | $CO_2Me$ | | (20.8) |
| | CN | | (19.1) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $RSCH_2CN$ | | |

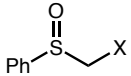
| R= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | Me | | (24.3) |
| | Et | | (24.0) |
| | *i*-Pr | | (23.6) |
| | *t*-Bu | | (22.9) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $PhSCH=CHCH_2SPh$ | | (26.3) |
| BuSH | 10-11 | (17.0) |
| PhSH | ≈7 | (10.3) |

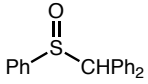
## SULFOXIDES



| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | H | | (35.1) |
| | Ph | | (29.0) |
| | SPh | | (29.0) |

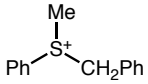


| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | H | | (33) |
| | Ph | | (27.2) |
| | SOPh | | (18.2) |

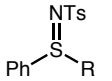


| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $Ph(CHPh_2)SO$ | | (24.5) |

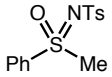
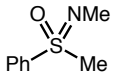
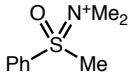
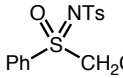
## SULFONIUM

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| $Me_3S^+=O$ | | (18.2) |
|  | | (16.3) |

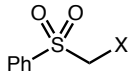
## SULFIMIDES & SULFOXIMINES



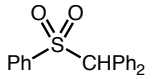
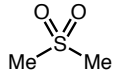
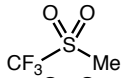
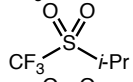
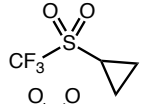
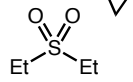
| R= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | Me | | (27.6) |
| | *i*-Pr | | (30.7) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
|  | | (24.5) |
|  | | (33) |
|  | | (14.4) |
|  | | (20.7) |

## SULFONES



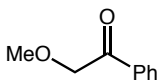
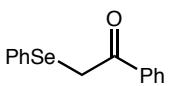
| X= | Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|---|
| | H | | (29.0) |
| | $CH_3$ | | (31.0) |
| | *t*-Bu | | (31.2) |
| | Ph | | (23.4) |
| | $CH=CH_2$ | | (22.5) |
| | CH=CHPh | | (20.2) |
| | CCH | | (22.1) |
| | CCPh | | (17.8) |
| | COPh | | (11.4) |
| | COMe | | (12.5) |
| | OPh | | (27.9) |
| | $N^+Me_3$ | | (19.4) |
| | CN | | (12.0) |
| | $NO_2$ | | (7.1) |
| | SMe | | (23.5) |
| | SPh | | (20.5) |
| | $SO_2Ph$ | | (12.2) |
| | $PPh_2$ | | (20.2) |

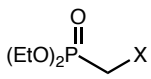
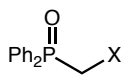
| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
|  | | (22.3) |
|  | | (31.1) |
|  | | (18.8) |
|  | | (21.8) |
|  | | (26.6) |
|  | | (32.8) |
| $(PhSO_2)_2CH_2Me$ | | (14.3) |

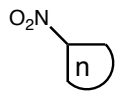
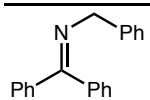
*Values <0 for $H_2O$ and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

# pKa's of CH bonds at Heteroatom Substituted Carbon & References



| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **ETHERS** | | |
| $CH_3OPh$ | | (49) |
| $MeOCH_2SO_2Ph$ | | (30.7) |
| $PhOCH_2SO_2Ph$ | | (27.9) |
| $PhOCH_2CN$ | | (28.1) |
|  | | (22.85) |
| **SELENIDES** | | |
|  | | (18.6) |
| $PhSeCHPh_2$ | | (27.5) |
| $(PhSe)_2CH_2$ | | (31.3) |
| $PhSeCH_2Ph$ | | (31.0) |
| $PhSeCH{=}CHCH_2SePh$ | | (27.2) |
| **AMMONIUM** | | |
| $Me_3N^+CH_2X$ | | |
| X= CN | | (20.6) |
| $SO_2Ph$ | | (19.4) |
| COPh | | (14.6) |
| $CO_2Et$ | | (20.0) |
| $CONEt_2$ | | (24.9) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **PHOSPHONIUM** | | |
| $P^+H_4$ | | -14 |
| $MeP^+H_3$ | | 2.7 |
| $Et_3P^+H$ | | 9.1 |
| $Ph_3P^+CH_3$ | | (22.4) |
| $Ph_3P^+i\text{-}Pr$ | | (21.2) |
| $Ph_3P^+CH_2COPh$ | | (6.2) |
| $Ph_3P^+CH_2CN$ | | (7.0) |
| **PHOSPONATES & PHOSPHINE OXIDES** | | |
|  | | |
| X= Ph | | (27.6) |
| CN | | (16.4) |
| $CO_2Et$ | | (18.6) |
| Cl | | (26.2) |
| $SiMe_3$ | | (28.8) |
|  | | |
| X= SPh | | (24.9) |
| CN | | (16.9) |
| **PHOSPHINES** | | |
| $Ph_2PCH_2PPh_2$ | | (29.9) |
| $Ph_2PCH_2SO_2Ph$ | | (20.2) |

| Substrate | pKa $H_2O$ | (DMSO) |
|---|---|---|
| **NITRO** | | |
| $RNO_2$ | | |
| R= $CH_3$ | ≈10 | (17.2) |
| $CH_2Me$ | | (16.7) |
| $CHMe_2$ | | (16.9) |
| $CH_2Ph$ | | (12.2) |
| $CH_2Bn$ | | (16.2) |
| $CH_2SPh$ | | (11.8) |
| $CH_2SO_2Ph$ | | (7.1) |
| $CH_2COPh$ | | (7.7) |
|  | | |
| n= 3 | | (26.9) |
| 4 | | (17.8) |
| 5 | | (16.0) |
| 6 | | (17.9) |
| 7 | | (15.8) |
| **IMINES** | | |
|  | | (24.3) |

Oxime ethers are ~ 10 pka units less acidic than their ketone counterparts Streitwieser, JOC 1991, 56, 1989

## REFERENCES


DMSO:

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JACS 105, 6188 (1983)
JOC 41, 1883 (1976)
JOC 41, 1885 (1976)
JOC 41, 2786 (1976)
JOC 41, 2508 (1976)
JOC 42, 1817 (1977)
JOC 42, 321 (1977)
JOC 42, 326 (1977)
JOC 43, 3113 (1978)
JOC 43, 3095 (1978)
JOC 43, 1764 (1978)
JOC 45, 3325 (1980)
JOC 45, 3305 (1980)
JOC 45, 3884 (1980)
JOC 46, 4327 (1981)
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Acc. Chem. Res. 21, 456 (1988)
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Unpublished results of W. P. Jencks

THF:
JACS 110, 5705 (1988)

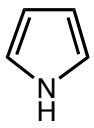

See cited website below for additional data

*Values <0 for $H_2O$ and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

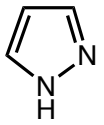
For a comprehensive compilation of Brodwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

# DMSO Acidities of Common Heterocycles

Bordwell, ACR, **1988**, *21*, 456
Bordwell http://www.chem.wisc.edu/areas/reich/pkatable/index.htm



23.0



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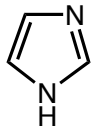
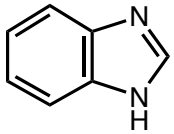


18.6



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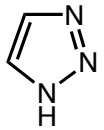

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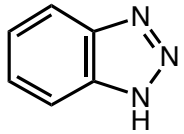
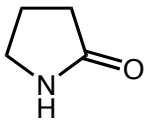


11.9

18.0



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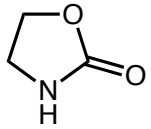

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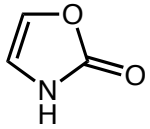

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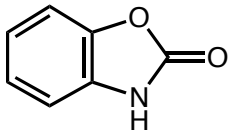
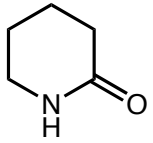
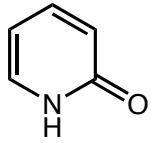


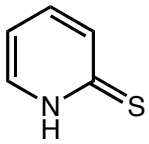
12.1



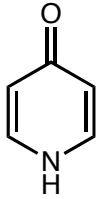
26.4



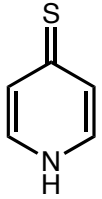
24.0



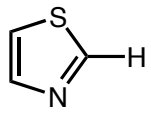
13.3



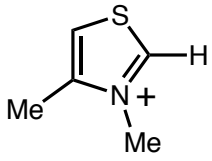
14.8



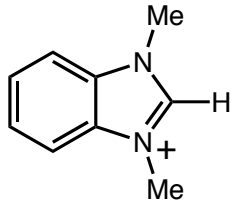
11.8



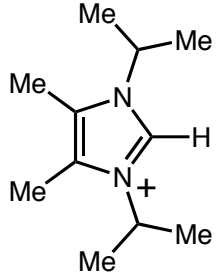
29.4



16.5



18.4



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***pKa Values***

**INDEX**



For complex chelating agents, see also reference 77.

Note. This document was compiled by W.P. Jencks and has been added to by F.H. Westheimer

## ACIDS

| Compound | pK | Ref. |
|---|---|---|
| $AgOH$ | 3.96 | 4 |
| $Al(OH)_3$ | 11.2 | 28 |
| $As(OH)_3$ | 9.22 | 28 |
| $H_3AsO_4$ | 2.22, 7.0, 13.0 | 28 |
| $H_2AsO_4^-$ | 6.98* | 77 |
| $HAsO_4$* | 11.53* | 77 |
| $As_2O_3$ | 0 | 4 |
| $H_3AsO_3$ | 9.22* | |
| $H_3BO_3$ | 9.23* | 28 |
| $H_2B_4O_7$ | 4.00 | 34 |
| $HB_4O_7$ | 9.00 | 34 |
| $Be(OH)_2$ | 3.7 | 4 |
| $HBr$ | -9.00 | 31 |
| $HOBr$ | 8.7 | 28 |
| $HOCl$ | 7.53, 7.46 | 28, 33 |
| $HClO_2$ | 2.0 | 28 |
| $HClO_3$ | -1.00 | 28 |
| $HClO_4$ (70%) | -10.00 | 31 |
| $CH_3SO_3H$ | -0.6 | 31 |
| $HCN$ | 9.40 | 34 |
| $H_2CO_3$ | 6.37, 6.35*, 3.58 | 34, 32 |
| $HCO_3$ | 10.33* | |
| $H_2CrO_4$ | -0.98 | 30 |
| $HCrO_4$ | 6.50* | 2, 30 |
| $HOCN$ | 3.92 | 34 |
| $HZ$ | 3.17*, 0.59* | 77 |
| $H_2GeO_3$ | 8.59, 12.72 | 34, 78 |
| $Ge(OH)_4$ | 8.68, 12.7 | 28 |
| $HI$ | -10.0 | 31 |
| $HOI$ | 11.0 | 28 |
| $HIO_3$ | 0.8 | 28 |
| $H_4IO_6^-$ | 6.00 | 34 |
| $H_5IO_6$ | 1.64, 1.55, 8.27 | 34, 28 |
| $HMnO_4$ | -2.25 | 30 |
| $NH_3OH$* | 5.98* | |
| $NH_4$* | 9.24* | 77 |
| $HN_3$ | 4.72* | 77 |
| $HNO_2$ | 3.29 | 28 |
| $HNO_3$ | -1.3 | 28 |
| $N_2H_5^+$ | 7.99* | 77 |
| $H_2N_2O_2$ | 7.05 | 34 |
| $H_2N_2O_2^-$ | 11.0 | 34 |
| $H_2OsO_5$ | 12.1 | 34 |
| $H_2O$ | 15.7 | none |
| $H_3O^+$ | -1.7 | none |
| $Pb(OH)_2$ | 6.48 (10.92) | 4 (78) |
| $H_3PO_2$ | 2.0, 2.23* | 28 |
| $H_2PO_4^-$ | 7.21* | 77 |
| $HPO_4$– | 12.32* | 77 |
| $H_3PO_3$ | 2.0 | 28 |
| $H_2PO_3^-$ | 6.58* | 77 |
| $H_4P_2O_7$ | 1.52* | 77 |
| $H_3\ P_2O_7^-$ | 2.36* | 77 |
| $H_2P_2O_7^=$ | 6.60* | 77 |
| $HP_2O_7^=$ | 9.25* | 77 |
| $HReO_4$ | -1.25 | 30 |
| $HSCN$ | 4.00 | 34 |
| $H_2SeO_3$ | 2.6, 8.3, 2.62* | 28 |
| $HSeO_3$ | 8.32 | 77 |
| $H_2SeO_4$ | Strong, 2.0 | 28 |
| $HSeO_4$ | 2.00 | 34 |
| $H_3SiO_3$ | 10.0 | 34 |
| $H_2SO_3$ | 1.9, 7.0, 1.76* | 28, 77 |
| $H_2SO_4$ | -3.0, 1.9 | 28 |
| $HSO_3$ | 7.21* | 77 |
| $HSO_4^-$ | 1.99* | 77 |
| $H_2S_2O_4$ | 1.9 | 29 |
| $H_2Se$ | 3.89* | 77 |
| $HSe^-$ | 11.00* | 77 |
| $H_2S$ | 7.00* | 77 |
| $HS^-$ | 12.92* | 77 |
| $HSbO_2$ | 11.0 | 34 |
| $HTe$ | 5.00 | 34 |
| $H_2Te$ | 2.64, 11.0 | 34, 78 |
| $H_2TeO_3$ | 2.7, 8.0 | 28 |
| $Te(OH)_6$ | 6.2, 8.8 | 28 |
| $H_2VO_4^-$ | 8.95 | 30 |
| $HVO_4^=$ | 14.4 | 30 |
| $H_2CrO_4$ | 0.74 | 77 |
| $HOCN$ | 3.73 | 77 |
| $HSCN$ | 0.85 | 77 |
| $H_3PO_2$ | 1.07 | 77 |
| $H_3PO_4$ | 2.12* | 77 |
| $H_2S_2O_3$ | 0.60*, 1.72* | 77 |
| $H_3AuO_3$ | 13.3, 16.0 | 78 |
| $H_3GaO_3$ | 10.32, 11.7 | 78 |
| $H_5IO_6$ | 3.29, 6.70, 15.0 (see above!) | 78 |
| $H_4V_6O_{17}$ | 1.96 | 78 |
| $H_2NSO_3H$ | 1.0 | 80 |

* *Indicates a thermodynamic value.*

## *PHOSPHATES AND PHOSPHONATES*

### Phosphates

| Compound | pK | Ref. |
|---|---|---|
| Phosphate | 1.97, 6.82, 12.5 | 55 |
| Glyceric acid 2-phosphate | 3.6, 7.1 | 53 |
| Enolpyruvic acid | 3.5, 6.4 | 53 |
| Methyl- | 1.54, 6.31 | 55 |
| Ethyl- | 1.60, 6.62 | 55 |
| n-Propyl- | 1.88,6.67 | 55 |
| n-Butyl- | 1.80, 6.84 | 55 |
| Dimethyl- | 1.29 | 55 |
| Di-n-propyl | 1.59 | 55 |
| Di-n-butyl- | 1.72 | 55 |
| Glucose-3- | 0.84, 5.67 | 56 |
| Glucose-4- | 0.84, 5.67 | 56 |
| α-glycero- | 1.40, 6.44 | 54 |
| β-glycero- | 1.37, 6.34 | 54 |
| 3-phosphoglyceric acid | 1.42, 3.42 | 54 |
| 2-phosphoglyceric acid | 1.42, 3.55, 7.1 | |
| peroxymonophosphoric acid | 4.05 | 69 |
| diphosphoglyceric acid | 7.40, 7.99 | 54 |
| glyceraldehyde- | 2.10, 6.75 | 54 |
| dioxyacetone- | 1.77,6.45 | 54 |
| hexose di- | 1.52, 6.31 | 54 |
| fructose-6- | 0.97, 6.11 | 54 |
| glucose-6- | 0.94, 6.11 | 54 |
| glucose-1- | 1.10, 6.13 | 54 |
| adenylic acid | 3.8?, 6.2? | 54 |
| inosinic acid | 2.4?, 6.4? | 54 |
| ADP | 2 strong, 6.6 | 54 |
| ATP | 3 strong, 6.6 | 54 |
| pyrophosphoric acid | 0.9, 2.0, 6.6, 9.4 | 54 |
| phosphopyruvic acid | 3.5, 6.38 | 54 |
| creatine phosphate | 2.7, 4.5 | 54 |
| arginine phosphate | 2.8, 4.5, 9.6, 11.2 | 54 |
| arginine | 2.02, 9.0, 12.5 | 54 |
| amino phosphate | (-0.9), 2.8, 8.2 | 54 |
| trimetaphosphate | 2.05 | 77 |

### Phosphonates

| | | |
|---|---|---|
| $H_2O_3P(CH_2)_4PO_3H_2$ | <2, 2.75, 7.54, 8.38 | 57 |
| $H_2O_3P(CH_2)_3PO_3H_2$ | <2, 2.65, 7.34, 8.35 | 57 |
| $H_2O_3PCH_2CH(CH_3)PO_3H_2$ | <2, 2.6, 7.00, 9.27 | 57 |
| $H_2O_3PCH_2PO_3H_2$ | <2, 2.57, 6.87, 10.33 | 57 |
| Methyl- | 2.35 | 57 |
| Ethyl- | 2.43 | 57 |
| n-propyl- | 2.45 | 57 |
| isopropyl- | 2.55, 7.75 | 57 |
| n-butyl- | 2.59, 8.19 | 57 |
| isobutyl- | 2.70, 8.43 | 57 |
| s-butyl- | 2.74, 8.48 | 57 |
| t-butyl- | 2.79, 8.88 | 57 |
| neopentyl- | 2.84, 8.65 | 57 |
| 1,1 Dimethylpropyl- | 2.88, 8.96 | 57 |
| n-hexyl- | 2.6, 7.9 | 57 |
| n-dodecyl- | --, 8.25 | 57 |
| $CH_3(CH_2)_5CH(COOH)$- | 1, -- | 57 |
| $CF_3$- | 1.16, 3.93 | 57 |
| $CCl_3$- | 1.63, 4.81 | 57 |
| $NH_3^+CH_2$- | 2.35, 5.9 | 57 |
| $(^-OOCCH_2)_2NH^+CH_2$- | --, 5.57 | 57 |
| $CHCl_2$- | 1.14, 5.61 | 57 |
| $CH_2CI$- | 1.40, 6.30 | 57 |
| $CH_2Br$- | 1.14, 6.52 | 57 |
| $(^-OOCCH_22NH^+(CH_2)_2$- | --, 6.54 | 57 |
| $CH_2I$- | 1.30, 6.72 | 57 |
| $NH_3^+CH_2CH_2$- | 2.45, 7.00 | 57 |
| $C_6H_5CH$=CH- | 2.00, 7.1 | 57 |
| $HOCH_2$- | 1.91, 7.15 | 57 |
| $C_6H_5NH_{2+}(CH_2)_3$- | 2.1, -- | 57 |
| $C_6H_5NH(CH_2)_3$- | --, 7.17 | 57 |
| $Br(CH_2)_2$- | 2.25, 7.3 | 57 |
| $CH_3(CH_2)_5CH(COO^-)$- | --, 7.5 | 57 |
| $C_6H_5CH_2$- | 2.3, 7.55 | 57 |
| $NH_3^+(CH_2)_4$)- | 2.55, 7.55 | 57 |
| $NH_3^+(CH_2)_5$- | 2.6, 7.6 | 57 |
| $NH_3^+(CH_2)_{10}$- | --, 8.00 | 57 |
| $^-OOC(CH_2)_{10}$- | --, 8.25 | 57 |
| $(CH_3)_3SiCH_2$- | 3.22, 8.70 | 57 |
| $C_6H_5CH_2$- | 3.3, 8.4 | 57 |
| $(C_6H_5)SC$- | 3.85, 9.00 | 57 |

### Arylphosphonic acids

$2X\text{-}RC_6H_3PO_3H_2$

| X | R | | |
|---|---|---|---|
| Cl | 4-$O_2N$ | 1.12, 6.14 | 57 |
| Br | 5-$O_2N$ | (a), 6.14 | 57 |
| Cl | 5-Cl | (a), 6.63 | 57 |
| Cl | H | 1.63, 6.98 | 57 |
| Br | H | 1.64, 7.00 | 57 |
| Br | 5-$CH_3$ | 1.81, 7.15 | 57 |
| Cl | 4-$NH_2$ | --, 7.33 | 57 |
| $CH_3O$ | 4-$O_2N$ | 1.53, 6.96 | 57 |
| $CH_3O$ | H | 2.16, 7.77 | 57 |
| $CH_3O$ | 4-$O_2N$ | --, 8.22 | 57 |
| HO | 4-$O_2N$ | 1.22, 5.39 | 57 |
| $O_2N$ | H | 1.45, 6.74 | 57 |
| F | H | 1.64, 6.80 | 57 |
| I | H | 1.74, 7.06 | 57 |
| $NH_2H$ | --, 7.29 | 57 | |
| $CH_3H$ | 2.10, 7.68 | 57 | |
| $C_6H_5$ | H | (a), 8.13 | 57 |
| HOOC | H | 1.71, 9.17 | 57 |

**These values were obtained in 50% ethanol.
(a) The compounds were not sufficiently soluble.
For graphical plots of a large number of substituted phosphorus compounds see 83.

| | | |
|---|---|---|
| triphosphate | 8.90, 6.26, 2.30 | 77 |
| tetrametaphosphate | 2.74 | 77 |

| | | | |
|---|---|---|---|
| fluorophosphate | 0.55, 4.8 | | 56 |

**Phosphonates (Ref. 2)**

| X | -H | -H | $-NH_3^+$ | $-NH_3^+$ |
|---|---|---|---|---|
| $X(CH_2)PO_3H_2$ | 2.35 | 7.1 | 1.85 | 5.35 |
| $X(CH_2)_2PO_3H_2$ | 2.45 | 7.85 | 2.45 | 7.00 |
| $X(CH_2)_4PO_3H_2$ | | | 2.55 | 7.55 |
| $X(CH_2)_5PO_3H_2$ | | | 2.6 | 7.65 |
| $X(CH_2)_6PO_2H_2$ | 2.6 | 7.9 | | |
| $X(CH_2)_{10}PO_2H_2$ | | | | 8.00 |

Phosphines in acetonitrile, see ref. 89.

## CARBOXYLIC ACIDS

### Aliphatic

| Compound | pK | Ref. |
|---|---|---|
| Acetoacetic | 3.58 | 6 |
| Acetopyruvic | 2.61, 7.85 (enol) | 6 |
| Aconitic, trans- | 2.80, 4.46 | 6 |
| Betaine | 1.84 | 6 |
| Citric | 3.09, 4.75, 5.41 | 6 |
| Crotonic | 4.69 | 6 |
| Dihydroxyfumaric | 1.14 | 6 |
| Dethylenediamine- | 2.00, 2.67 | 6 |
| tetraacetic | 6.16, 10.26 | |
| Formic | 3.77* | 2 |
| Fumaric | 3.03, 4.54 | 6 |
| Glyceric | 3.55 | 6 |
| Glycollic | 3.82 | 6 |
| Glyoxylic | 3.32 | 6 |
| Homogentistic | 4.40 | 6 |
| α-keto-β-methyl valeric | 2.3 | 6 |
| Lactic | 3.86 | 6 |
| Maleic | 1.93, 6.58 | 6 |
| Malic | 3.40, 5.2 | 6 |
| Oxaloacetic (trans-enol) | 2.56 | 6 |
| +(cis-enol) | 2.15, 4.06 | 6 |
| Protocatechuic | 4.48 | 6 |
| Pyruvic | 2.50 | 6 |
| Tartaric + | 2.99, 4.40 | 6 |
| + or - | 2.89, 4.40 | 6 |
| meso | 3.22, 4.85 | 6 |
| Vinylacetic | 4.42 | 6 |

### Acetic acids, substituted

| | | |
|---|---|---|
| H- | 4.76* | 20 |
| $O_2N$- | 1.68* | 20 |
| $(CH_3)_3N^+$- | 1.83* | 20 |
| $(CH_3)_2NH^+$- | 1.95* | 20 |
| $CH_3NH_2^+$- | 2.16* | 20 |
| $NH_3^+$- | 2.31* | 20 |
| $CH_3SO_2$- | 2.36* | 20 |
| NC- | 2.43* | 20 |
| $C_6H_5SO_2$- | 2.44 | 20 |
| $HO_2C$ | 2.83* | 20 |
| $C_6H_5SO$- | 2.66 | 20 |
| F- | 2.66 | 20 |
| Cl- | 2.86* | 20 |
| Br- | 2.86 | 20 |
| $Cl_2$- | 1.29 | 20 |
| $F_2$- | 1.24 | 20 |
| $Br_3$- | 0.66 | 20 |
| $Cl_3$- | 0.65 | 20 |
| $F_3$- | 0.23 (-0.26) (2) | 20 |
| $HONC_4$ | 3.01 | 20 |
| $F_3C$- | 3.07* | 20 |
| $N_3$- | 3.03 | 20 |
| I- | 3.12 | 20 |
| $C_6H_5O$- | 3.12 | 20 |
| $C_2H_5O_2C$- | 3.35 | 20 |
| $C_6H_5S$- | 3.52* | 20 |
| $CH_3O$- | 3.53 | 20 |
| NCS- | 3.58 | 20 |
| $CH_3CO$- | 3.58* | 20 |
| $C_2H_5O$- | 3.60 | 20 |
| n-$C_3H_7O$ | 3.65 | 20 |
| n-$C_4H_9O$ | 3.66 | 20 |
| sec.-$C_4H_9O$- | 3.67 | 20 |
| HS- | 3.67* | 20 |
| i-$C_3H_7O$- | 3.69* | 20 |
| $CH_3S$- | 3.72* | 20 |
| i-$C_3H_7S$- | 3.72* | 20 |
| $C_6H_5CH_2S$- | 3.73* | 20 |
| $C_2H_5S$- | 3.74* | 20 |
| n-$C_3H_7S$- | 3.77* | 20 |
| n-$C_4H_9S$- | 3.81* | 20 |
| HO- | 3.83* | 20 |
| $^-O_3S$- | 4.05 | 20 |
| $(C_6H_5)_3CS$- | 4.30* | 20 |
| $C_6H_5$- | 4.31* | 20 |
| $CH_2$-CH- | 4.35* | 20 |

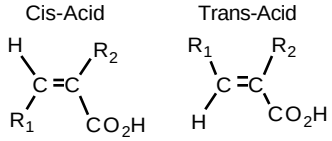
** Indicates thermodynamic values.*

**Unsaturated acids (25°)**

| Compound | pK | ref. |
|---|---|---|
| trans-$CH_3$-CH=$CHCO_2H$ | 4.69* | 20 |
| cis-$CH_3$-CH=$CHCO_2H$ | 4.44* | 2 |
| $C_6H_5$-$CH_2CH_2CO_2H$ | 4.66* | 2 |
| trans-$C_6H_5$-CH=$CHCO_2H$ | 4.44* | 2 |
| m-$CH_3OC_6H_4CH_2CH_2CO_2H$ | 2 | 4.65* |
| m-$CH_3OC_6H_4CH$=$CHCO_2H$ | 4.38* | 2 |
| m-$ClC_6H_4CH_2CH_2CO_2H$ | 4.58* | 2 |

| Compound | pK | ref. |
|---|---|---|
| H-$CH_2CH_2CO_2H$ | 4.88* | 2 |
| H-CH=$CHCO_2H$ | 4.25* | 2 |
| $C_6H_5CH_2CH_2CO_2H$ | 4.66* | 2 |
| $C_6H_5$CH=$CHCO_2H$** | 4.44* | 2 |
| $C_6H_5CH_2CH_2CO_2H$ | 4.66* | 2 |
| $C_6H_5$CH=$CHCO_2H$** | 4.44 | 2 |
| m-$ClC_6H_4$CH=$CHCO_2H$** | 4.29* | 2 |

**Unsaturated acids, *Cis*- and *Trans*-**




| $R_1$ | $R_2$ | cis-acid | trans-acid | Ref. |
|---|---|---|---|---|
| H- | H- | 4.25* | 4.25* | 2 |
| $CH_3$- | H- | 4.44* | 4.69* | 2 |
| Cl- | H- | 3.32 | 3.65 | 2 |
| $C_6H_5$- | H- | 3.88* | 4.44* | 2 |
| $ClC_6H_4$ | H- | 3.91 | 4.41 | 2 |
| 6-$BrC_6H_4$ | H- | 4.02 | 4.41 | 2 |
| $CH_3$- | $CH_3$- | 4.30 | 5.02 | 2 |
| $C_6H_5$- | H- | 5.26*** | 5.58*** | 2 |
| 2,4,6-$(CH_3)_3C_6H_2$- | H- | 6.12*** | 5.70*** | 2 |
| $C_6H_5$- | $CH_3$- | 4.98*** | 5.98*** | 2 |

**Dicarboxylic acids, unsaturated***

| | | |
|---|---|---|
| Maleic | 1.92, 6.23 | 2 |
| Citraconic (Dimethylmaleic acid) | 2.29, 6.15 | 2 |
| Acetylenedicarboxylic | 1.73, 4.40 | 2 |
| $\Delta^1$-tetrahydrophthalic | 3.01, 5.34 | 2 |
| Bromomaleic | 1.45, 4.62 | 2 |
| Bromofumaric | 1.46, 3.57 | 2 |
| Chlorofumaric | 1.78, 3.81 | 2 |
| Fumaric | 3.02, 4.38 | 2 |
| Mesaconic (Dimethylfumaric acid) | 3.09, 4.75 | 2 |
| Phthalic | 2.95, 5.41 | 2 |
| Itaconic (1-Propene-2-3-dicarboxylic acid) | 3.85, 5.45 | 2 |
| Chloromaleic | 1.72, 3.86 | 2 |

**Alicyclic Dicarboxylic acids**

| | | |
|---|---|---|
| cis-Caronic(1,1-dimethylcyclopropane-23-dicarboxylic acid | 2.34*, 8.31* | 2 |
| 1,2-trans-cyclopropanedicarboxylic | 3.65*, 5.13* | 2 |
| trans-caronic | 3.82*, 5.32* | 2 |
| 1,2-cis-cyclopropane-dicarboxylic | 3.33*, 6.47* | 2 |

**trans
***in 40% acetone
*thermodynamic

**Aliphatic**

Alicyclic Dicarboxylic acids

| Compound | pK | Ref | Compound | pK | Ref |
|---|---|---|---|---|---|
| 1,2-trans-Cyclopropane-dicarboxylic | 3.65, 5.13 | 2 | cis-Ethyleneoxide-dicarboxylic | 1.94, 3.92 | 2 |
| trans-Ethyleneoxide-dicarboxylic | 1.93, 3.25 | 2 | 1,3-cis-Cyclobutane-dicarboxylic | 4.03, 5.31 | 2 |
| 1,3-trans -Cyclobutanedi-carboxylic | 3.81, 5.28 | 2 | 1,2-cis-Cyclopentane-dicarboxylic | 4.37, 6.51 | 2 |
| 1,2-trans-Cyyclopentane-dicarboxylic | 3.89, 5.91 | 2 | 1,3-cis-Cyclopentane dicarboxylic | 4.23, 5.53 | 2 |
| 1,3-trans-Cyclopentane-dicarboxylic | 4.40, 5.45 | 2 | 1,2-cisCyclohexane-dicarboxylic | 4.34, 6.76 | 2 |
| 1,2-trans-Cyclohexane-dicarboxylic | 4.18, 5.93 | 2 | 1,3 -cis-Cyclohexane-dicarboxylic | 4.10, 5.46 | 2 |
| 1,3-trans-Cyclohexane-dicarboxylic | 4.31, 5.73 | 2 | 1,4-cis-Cyclohexane di-carboxylic | 4.44, 5.79 | 2 |
| 1,4-trans-Cyclohexane-dicarboxylic | 4.18, 5.42 | 2 | | | |

**Dicarboxylic acids***

| | | | | | |
|---|---|---|---|---|---|
| oxalic | 1.23, 4.19 | 2 | Succinic | 4.19, 5.48 | 2 |
| Malonic | 2.83, 5.69 | 2 | O-O'-Dimethyl- | 3.77, 5.94 | 2 |
| Methyl- | 3.05, 5.76 | 2 | (high melting) | | |
| Ethyl- | 2.99, 5.83 | 2 | O-O'-Dimethyl- | 3.94, 6.20 | 2 |
| n-propyl | 3.00, 5.84 | 2 | (low melting) | | |
| i-propyl- | 2.94, 5.88 | 2 | O,O'-Diethyl- | 3.63, 6.46 | 2 |
| Dimethyl- | 3.17, 6.06 | 2 | (high melting) | | |
| Methylethyl- | 2.86, 6.41 | 2 | O,O'-Diethyl- | 3.51, 6.60 | 2 |
| Diethyl- | 2.21, 7.29 | 2 | (low melting) | | |
| Ethyl-n-propyl- | 2.15, 7.43 | 2 | Tetramethyl- | 3.50, 7.28 | 2 |
| Di-n-propyl- | 2.07, 7.51 | 2 | | | |
| Glutaric | 4.34, 5.42 | 2 | Adipic | 4.42, 5.41 | 2 |
| B-Methyl | 4.25, 6.22 | 2 | Pimelic | 4.48, 5.42 | 2 |
| B-Ethyl | 4.29, 6.33 | 2 | Suberic | 4.52, 5.40 | 2 |
| B-n-Propyl | 4.31, 6.39 | 2 | Azelaic | 4.55, 5.41 | 2 |
| B,B-Dimethyl- | 3.70, 6.29 | 2 | DL-1:2-Dichlorosuccinic | 1.68, 3.18 | 20 |
| B,B-Methylethyl- | 3.62, 6.70 | 2 | meso-1:2-Dichlorosuccinic | 1.74, 3.24 | 20 |
| B,B-Diethyl- | 3.62, 7.12 | 2 | DL-1:2-Dibromosuccinic | 1.48, ---- | 20 |
| B,B-Di-n-propyl | 3.69, 7.31 | 2 | meso-1:2-Dibromosuccinic | 1.42, 2.97 | 20 |
| D-Tartaric | 3.03, 4.45 | 20 | DL-1:2-Dimethylsuccinic | 3.93, 6.00 | 20 |
| DL-Tartaric | 3.03, ---- | 20 | meso-1:2-Dimethylsuccinic | 3.77, 5.36 | 20 |
| meso-Tartaric | 3.29, 4.92 | 20 | | | |

**All are thermodynamic values*

**Aliphatic**

**Bicyclo[2.2.2]octane-1-carboxylic acids, 4-substituted**

| | | |
|---|---|---|
| H- | 6.75 | 2 |
| $C_2H_5O_2C$- | 6.31 | 2 |
| NC- | 5.90 | 2 |
| HO- | 6.33 | 2 |
| Br- | 6.08 | 2 |

**Lysergic acid, etc.**

| | | |
|---|---|---|
| ergometrine | 6.8, -- | 2 |
| Dihydroergometrine | 7.4, -- | 2 |
| β-dihydrolysergol | 8.2, -- | 2 |

| | | |
|---|---|---|
| Lysergic acid | 7.8, 3.3 | 2 |
| α-dihydrolysergic | 8.3, 3.6 | 2 |
| ergometrinine | 7.3, -- | 2 |
| α-dihydrolysergol | 8.3, -- | 2 |
| 6-methylergoline | 8.85, -- | 2 |
| isolysergic acid | 8.4, 3.4 | 2 |
| γ-dihydrolysergic | 8.6, 3.6 | 2 |

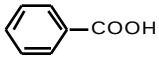
**Hydroxycyclohexanecarboxylic acids**

| | | |
|---|---|---|
| Cyclohexanecarboxylic | 4.90 | 2 |
| cis-1,2 | 4.80 | 2 |
| cis-1,3 | 4.60 | 2 |
| cis-1,4 | 4.84 | 2 |
| trans-1,2 | 4.68 | 2 |
| trans-1,3 | 4.82 | 2 |
| trans-1,4 | 4.68 | 2 |

**Aromatic**

| | | |
|---|---|---|
| benzene-$CO_3H$ | 4.20* | 2 |
| Anthracene-1-COOH | 3.69 | 2 |
| Anthracene-9-COOH | 3.65 | 2 |
| naphthalene-2-COOH | 4.17 | 2 |
| Naphthalene-1-COOH | 3.69 | 2 |

**Substituted benzoic acids (ref. 2)**




| **Benzoic acid** | **o** | **m** | **p** |
|---|---|---|---|
| H- | 4.20* | 4.21* | |
| $O_2N$- | 2.17* | 3.45* | 3.44 |
| $CH_3CO$- | | | |
| $CH_3SO_2$- | | 3.64* | 3.52* |
| $CH_3S$- | | | |
| HS- | | | |
| Br- | 2.85* | 3.81* | 4.00* |
| F- | 3.27* | 3.87* | 4.14* |
| $CH_3O$- | 4.09* | 4.09* | 4.47* |
| n-$C_3H_7O$- | 4.24* | 4.20* | 4.46* |
| n-$C_4H_9O$- | | 4.25* | 4.53* |

| **Benzene Polycarboxylic acids** | **Ref. 2** |
|---|---|

| **Acid** | **Position of carboxyl** | **$pK^I$** | **$pK^{II}$** | **$pK^{III}$** | **$pK^{IV}$** | **$pK^V$** | **$pK^{VI}$** |
|---|---|---|---|---|---|---|---|
| Benzoic | 1 | 4.17* | | | | | |
| Phthalic | 1,2 | 2.98* | 5.28* | | | | |
| Isophthalic | 1,3 | 3.46* | 4.46* | | | | |
| Terephthalic | 1,4 | 3.51* | 4.82* | | | | |
| Hemimellitic | 1,2,3 | 2.80* | 4.20* | 5.87* | | | |
| Trimellitic | 1,2,4 | 2.52* | 3.84* | 5.20* | | | |

| | | | |
|---|---|---|---|
| $C_6H_5O$- | 3.53* | 3.95* | 4.52* |
| $CH_3$- | 3.91* | 4.24* | 4.34* |
| $(CH_3)_2CH$- | | | 4.35* |
| $(CH_3)_3N^+$- | 1.37 | 3.45 | 3.43 |
| NC- | | 3.60* | 3.55* |
| $HO_2C$* | 2.95* | 3.54 | 3.51 |
| $F_3C$- | | 3.79 | |
| HO- | 2.98* | 4.08* | 4.58* |
| I- | 2.85* | 3.86* | |
| Cl- | 2.94* | 3.83* | 3.99* |
| $(CH_3)_3Si$- | | 4.24* | 4.27* |
| $C_2H_5O$- | 4.21* | 4.17* | 4.45* |
| i-$C_3H_7O$- | 4.24* | 4.15* | 4.68* |
| n-$C_5H_{11}O$- | | | 4.55* |
| $C_6H_5$- | 3.46* | | |
| $CH_3CH_2$- | 3.77 | | 4.35* |
| $(CH_3)_3C$- | 3.46 | 4.28 | 4.40* |
| $^-HO_3P$- | 3.78 | 4.03 | 3.95 |
| $^-O_3S$- | | 4.15 | 4.11 |
| $H_2N$- | 4.98 | 4.79 | 4.92 |
| $(CH_3)_2N$- | 8.42 | 5.10 | 5.03 |
| $^-HO_3As$- | | | 4.22 |
| $^-O_2C$- | 5.41** | 4.60 | 4.82 |
| $CH_3NH$- | 5.3 | 5.10 | 5.04 |

*thermodynamic
for complex chelating agents, see also ref. 84.
see also page 9a for more carboxylic acids.

**Ortho-substituted benzoic acids**

| **Benzoic acid** | **pK** | **Ref.** |
|---|---|---|
| 2-$CH_3$- | 3.91** | 2 |
| 2-t-$C_4H_9$- | 3.46 | 2 |
| 2,6-$(CH_3)_2$- | 3.21 | 2 |
| 2,3,4,6-$(CH_3)_4$- | 4.00 | 2 |
| 2,3,5,6-$(CH_3)_4$- | 3.52 | 2 |
| 2-$C_2H_5$- | 3.77 | 2 |
| 2-$C_6H_5$- | 3.46** | 2 |
| 2,4,6-$(CH_3)_3$- | 3.43 | 2 |
| 2,3,4,5-$(CH_3)_4$- | 4.22 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Trimesic | 1,3,5 | 3.12* | 3.89* | 4.70* | | |
| Mellophanic | 1,2,3,4 | 2.06* | 3.25* | 4.73* | 6.21* | |
| Prehnitic | 1,2,3,5 | 2.38* | 3.51* | 4.44* | 5.81* | |
| Pyromellitic | 1,2,4,5 | 1.92* | 2.87* | 4.49* | 5.63* | |
| Benzenepentacarboxylic | 1,2,3,4,5 | 1.80* | 2.73* | 3.97* | 5.25* | 6.46* |
| Mellitic | 1.2,3,4,5,6 | 1.40* | 2.19* | 3.31* | 4.78* | 5.89* 6.96* |

**ionic strength 0.03*
***thermodynamic*

| **Carboxylic Acids** | **Ref. 77** |
|---|---|
| Aminomalonic acid* | 3.32, 9.83 |
| N-Butylaminoacetic acid | 2.29, 10.07 |
| 2-carboxyethyliminodiacetic acid | 2.06, 3.69, 9.66 |
| β-carboxymethylaminopropionic | 3.61, 9.46 |
| α,α-diaminobutyric | 1.85, 8.24, 10.44 |
| Di-(carboxymethyl)-aminomethyl phosphonic acid | 2.00, 2.25, 5.57, 10.76 |
| α,β-dimercaptosuccinic | 2.40, 3.46, 9.44, 11.82 |
| Ethylenediamine-N,N-diacetic | 5.58, 11.05 |
| α-hydroxybutyric | 3.65 |
| N-2-hydroxyethyliminodiacetic | 2.2, 8.73 |
| 3-hydroxypropyliminodiacetic | 2.06, 9.24 |
| Iminodipropionic | 4.11, 9.61 |
| Isobutyric* | 4.86 |
| Mandelic acid | 3.41 |
| 2-Mercaptoethyliminodiacetic | -2.14, 8.17, 10.79 |
| Methyliminodiacetic | 2.81, 10.18 |
| 2-Methoxyethyliminodiacetic | 2.2, 8.96 |
| 2-Methylthioethyliminodiacetic | 2.1, 8.91 |
| oxalic acid* | 1.25, 4.14 |
| N-n-propylaminoacetic | 2.25, 10.03 |
| N-2-sulfoethyliminodiacetic | 1.92, 2.28, 8.16 |
| α-Bromobutyric acid | 2.97 |
| N-(carbamoylmethyl)-imino-diacetic acid | 2.30, 6.60 |
| Cyanomethyliminodiacetic | 3.06, 4.34 |
| α,β-diaminopropionic acid | 1.23, 6.69 |
| Diethylaminoacetic | 2.04, 10.47 |
| Dimethylaminoacetic | 2.08, 9.80 |
| N-ethylaminoacetic | 2.30, 10.10 |
| Gluconic* | 3.86 |
| β-hydroxybutyric | 4.39 |
| β-hydroxypropionic | 3.73 |
| Iminodiacetic* | 2.98, 9.89 |
| β-iodopropionic* | 4.04 |
| N-isopropylaminoacetic | 2.36, 10.06 |
| α-mercaptobutyric | 3.53 |
| N-methylaminoacetic | 2.24, 10.01 |
| Nitrilotriacetic | 3.03, 3.07, 10. |
| 2-Phosphonoethyliminodiacetic | 1.95, 2.45, 6.54, 10.46 |

**Thermodynamic*

**PHENOLS**

| Compound | pK | Ref. | Compound | pK | Ref. |
|---|---|---|---|---|---|
| Chromotropic acid | 5.36, 15.6 | 6 | Resorcinol | --, 9.15 (30°) | 50 |
| o-Methoxyphenol | --, 9.93 | 50 | p-Methoxyphenol | --, 10.16 | 50 |
| o-Hydroxybenz-aldehyde | 7.95 | 50 | 3-Hydroxyanthranilic acid | 10.09, 5.20 | 51 |
| 2-Amino-4,5 dimethylphenol hydrochloride | 10.4 5.28 | 51 | 2-Aminophenol hydrochloride | 9.99, 4.86 | 51 |
| 4,5-dihydroxybenzene-1,3 disulphonic acid | 7.66 12.6e | | | | |
| Kojic acid | 9.40 | 77 | | | |

| Phenol | o | m | p | Phenol | o | m | p |
|---|---|---|---|---|---|---|---|
| H- | 9.95* | 9.94* | | $O_2N$- | 7.23* | 8.35* | 7.14* |
| $(CH_3)_3N^+$- | 7.42 | 8 | 8 | OCH- | 6.79 | 8.00 | 7.66 |
| $CH_3SO_2$- | | 9.33 | 7.83 | NC- | | 8.61** | 7.95 |
| $CH_3CO$- | | 9.19 | 8.05 | $CH_3O_2C$- | | | 8.47* |
| $C_2H_5O_2C$- | | | 8.50* | n-$C_4H_9O_2C$- | | | 8.47* |
| $C_3H_5CH_2O_2C$- | | | 8.41* | I- | | 9.17* | |
| Br- | 8.42* | 9.11* | 9.34* | Cl- | 8.48* | 9.02* | 9.38* |
| F- | 8.81* | 9.28* | 9.95* | $CH_3S$- | | 9.53 | 9.53 |
| HO- | 9.48 | 9.44 | 9.96 | $HOCH_2$- | 9.92* | 9.83* | 9.82* |
| $CH_3$- | 10.28* | 10.08 | 10.19* | $C_2H_5$- | 10.2 | 9.9 | 10.0 |
| $CH_3O$- | 9.93 | 9.65 | 10.20 | $H_2N$- | 9.71 | 9.87 | 10.30 |
| $^-O_2C$- | | 9.94* | 9.39* | $^-O_3S$- | | 9.29 | 9.03 |
| $^{--}O_3P$- | | 10.2 | 9.9 | $^{--}O_3As$ | | | 8.37 |
| $C_6H_5$- | 9.93 | 9.59 | 9.51 | NO- | | | 6.35** |
| 2-Chloro-4-Nitro- | | 5.42 | 79 | | | | |
| 2-Nitro-4-Chloro- | | 6.46 | 79 | | | | |

** Thermodynamic*
***Reference 52*

## ALCOHOLS and other OXYGEN ACIDS

### Alcohols

| Compound | pK | Ref. |
|---|---|---|
| Choline | 13.9 | 6 |
| Chloral hydrate | 9.66, 11.0 | 61 |
| Trifluoroethanol | 12.5 | 62 |
| $CF_3CH_2OH$ | 11.4, 12.43 | 63 |
| $CF_3CH(OH)CH_3$ | 11.8 | 63 |
| $CF_3CH_2(CH_3)3OH$ | 12.43 | 10 |
| $C_3F_7CH_2OH$ | 11.4** | 63 |
| $(C_3F_7)_2CHOH$ | 10.6** | 63 |
| $HCCCH_2OH$ | 13.55 | 64 |
| $C(CH_2OH))_4$ | 14.1 | 64 |
| $HOCH_2CHOHCH_2OH$ | 4.4 | 64 |
| $HOCH_2CH_2OH$ | 14.77 | 64 |
| $CH_3CCH_2OH$ | 14.82 | 64 |
| $CH_3OH$ | 15.54 | 64 |
| $CH_2=CHCH_2OH$ | 15.52 | 64 |
| $H_2O$ | 15.74 | 64 |
| $CH_3CH_2OH$ | 16 | 64 |

**Substituent effects for ionization of $RCH_2OH$**

| R | | | |
|---|---|---|---|
| $CCl_3$- | 12.24,11.80 | | 64,65 |
| CF3- | 12.37 | | 64 |
| $CHF_2CH_2$- | 12.74 | | 64 |
| $CHCl_2$- | 12.89 | | 64 |
| CHEC- | 13.55 | | 64 |
| $H_2Cl$- | 14.31 | | 64 |
| $CH_3CCH_2$- | 14.8 | | 64 |
| $HOCH_2$ | 15.1 | | 64 |
| H- | 15.5 | | 64 |
| $CH_2=CH$- | 15.5 | | 64 |
| $CH_3$-(extrap) | (15.9) | | 64 |
| $CF_3C(CH_3)_2OH$ | 11.6 | | 64 |
| $HOCH_2CF_2CH_2OH$ | 11 | | 64 |
| Primary alcohols=R•$CH_2$•OH and Secondary alcohols in 50% alcohol | | | |
| $C_2F_5$ | 11.35 | | 65 |
| $C_4F_9$ | 11.35 | | 65 |
| $C_5F_{11}$ | 11.37 | | 65 |
| $C_7F_{15}$ | 11.35 | | 65 |
| $CHF_2$ | 12.00 | | 65 |
| $CF_2Cl$ | 11.63 | | 65 |
| $CHF_2CF_2$ | 11.34 | | 65 |
| $CHF_2$ • $(CF_2)_2$ | 11.35 | | 65 |
| CF3 • CH2 | 12.7 | | 65 |
| $CF_3$ • $(CH_2)_2$ | 12.9 | | 65 |
| $CF_3$ • CHMe • OH | 11.28 | | 65 |
| $C_3F_7$ • CHMe • OH | 11.38 | | 65 |
| $C_3F_7CHEt$ • OH | 11.37 | | 65 |
| $C_3F_7CHPr$ • OH | 11.37 | | 65 |
| $C_3F_7$ • $CH(CF_3)$ • OH | 10.46 | | 65 |
| $C_3F_7$•$CH(C_2F_5)$•OH | 10.48 | | 65 |
| $(C_3F_7)_2CH$•OH | 10.52 | | 65 |

### Carbonium ions

| Triphenylmethanols in | $H_2SO_4$ | $HC1O_4$ | $HNO_3$ | ref | |
|---|---|---|---|---|---|
| 4,4,4-Trimethoxy | | .82. | .82 | .80 | 66 |
| 4,4'-Dimethoxy | -1.24 | -1.14 | -1.11 | 66 | |
| 4-Methoxy | -3.40 | -3.59 | -3.41 | 66 | |
| 4-Methyl | -5.41 | -5.67 | | 66 | |
| 4_Trideuteriomethyl- | 5.43 | 5.67 | | 66 | |
| 3,3',3"-Trimethyl- | 6.35 | -5.95 | | 66 | |
| **Unsubstituted triphenyl-** | | | | | |
| methanol- | 6.63 | -6.89 | 6.60 | 66 | |
| 64 4,4;,4;-Trichloro- | | | 7.74- | 8.01 | 66 |
| 64 4_Nitro- | | | 9.15- | 9.76 | 66 |

| | | |
|---|---|---|
| $CCl_3CH_2OH$ | 11.8*** | |
| $CF_3CH_2OH$ | 11.3*** | |

### Hydroxamic acids

| | | | | |
|---|---|---|---|---|
| Furo- | 8.45 | | 72 | |
| Glycine | 7.40 | | 72 | |
| Hippuro- | 8.80 | | 72 | |
| *iso*Nicotin | 7.85 | | 72 | |
| 64 p-Methylbenz- | | 8.90 | | 72 |
| Nicotin- | | 8.30 | | 72 |
| Nicotin-methiodide | 6.46 | | 72 | |
| *m*-Nitrobenz- | 8.07 | | 72 | |
| Picolin | 8.50 | | 72 | |
| Pyrimidine-2-carbox- | 7.88 | | 72 | |
| Salicyl- | 7.43 | | 72 | |
| Tropo- | | 9.09 | | 72 |

### Other oxygen acids

| | | | | |
|---|---|---|---|---|
| Trimethylamine-n-oxide | 4.6 | | 18 | |
| Dimethylglyoxime (50% dioxane) | | 12.84 | | 77 |
| O-methyl ether | 12.92 | | 77 | |
| Tropolone | 12a | | 77 | |
| α-Bromotropolone | 6.95[a] | | 77 | |
| Acetald hydrate | 13.48 | | 91 | |
| Formald hydrate | 13.29 | | 91 | |

[a]50% dioxane
***50 aquaeous ethanol

## OTHER OXYGEN ACIDS

| Compound | pK | Ref. |
|---|---|---|
| **Pyridine oxides** | | |
| 4-Aminopyridine 1-oxide | 3.69 | 67 |
| 4-Dimethylaminopyridine 1-oxide | 3.88 | 67 |
| 4-Dimethylaminopyridine 1-oxide | 3.88 | 67 |
| 4-Dimethylamino-1-methoxypyridinium perchlorate | >11 | 67 |
| 2-Methylaminopyridine 1-oxide | 2.61 | 67 |
| 2-Amino-1-methoxypyridinium perchlorate | 12.4 | 67 |
| 4-Hydroxypyridine 1-oxide | 2.45 | 67 |
| 4-Methoxypyridine 1-oxide | 2.05 | 67 |
| 1-Methoxypyridi-4-one | 2.57 | 67 |
| 2-Hydroxypyridine 1-oxide | -0.8 | 67 |
| 2-Ethoxypyridine 1-oxide | 1.18 | 67 |
| 1-Methoxypyrid-2-one | -1.3 | |
| 4-Methylaminopyridine 1-oxide | 3.85 | 67 |
| 4-Amino-1-methoxypyridinium perchlorate | >11 | 67 |
| 2-Aminopyridine 1-oxide | 2.67 | 67 |
| 2-Dimethylaminopyridine 1-oxide | 2.27 | 67 |
| 2-Methylamino-1-methoxypyridinium toluene-p-sulphonate | >11 | 67 |
| 4-Benzyloxypyridine 1-oxide | 1.99 | 67 |
| 1-Benzyloxypyrid-4-one | 2.58 | 67 |
| 2-Methoxypyridine 1-oxide | 1.23 | 67 |
| 1-Benzyloxypyrid-2-one | -1.7 | 67 |

**Pyridine 1-oxides**

| R | pK | Ref. |
|---|---|---|
| 4-$CH_3$ | 1.29 | 47 |
| 3-$CH_3$ | 1.08 | 47 |
| 3,4-$(CH)_4$ | 1.01 | 47 |
| 3-$COOC_4H_9$ | 0.03 | 47 |
| 4-$NO_2$ | -1.7 | 47 |
| 3-$NH_2$ | 1.47 | 47 |
| H | 0.79 | 47 |
| 3-COOH | 0.09 | 47 |
| 4-COOH | -0.48 | 47 |

**Peroxides ROOH (Ref. 70)**

| H | $CH_3$ | $C_2H_5$ | iso-$C_3H_7$ | tert-$C_4H_9$ | iso-$C_4H_9$ |
|---|---|---|---|---|---|
| 11.6 | 11.5 | 11.8 | 12.1 | 12.8 | 12.8 |

| **Oximes** | ref. 93 |
|---|---|
| benzoquinoline mon- | 6.25 |
| 3-pyridine-1,2-ethanedione-2-oxime methiodide | 7.20 |
| Pyridine-2-aldoxime heptiodide | 8.00 |
| Pyridine-4-aldoxime methiodide | 8.50 |
| Pyridine-4-aldoxime pentiodide | 8.50 |

| **Hydroxamic acids** | | |
|---|---|---|
| Aceto- | 9.40 | 68 |
| n-Butyro- | 9.48 | 68 |
| n-Butyro- | 9.00 | 68 |
| p-Methoxybenzo- | 9.19 | 68 |
| N-Hydroxyphthalimide | 7.00, 6.10 | 71, 72 |
| Salicylo | 7.32 | 68 |
| Benzo- | 8.88 | 68 |
| p-Chlorobenzo- | 9.59 | 68 |
| α-Naphtho- | ~7.7 | 68 |
| Propiono- | 9.46 | 68 |

| **Oximes** | | |
|---|---|---|
| Benzophenone oxime | 11.3 | 18 |
| Diethyl ketoxime | 12.6 | 18 |
| Isonitrosoacetylacetone (INAA) | 7.4 | 76 |
| 5-Methyl-1,2,3-cyclohexanetrione-1,3-dioxime | 8.3 | 76 |
| Acetophenone oxime | 11.48 | 18 |
| Acetoxime | 11.42 | 18 |
| Isonitrosoacetone (INA) | 8.3 | 76 |
| Salicyclaldoxime (SA) | 9.2 | 76 |
| 1,2,3-Cyclohexanetrionetrioxime | 8.0 | 76 |
| 5-Methyl-1,2,3-cyclohexane-trionetrioxime | 8.0 | 76 |

| **Oxygen acids** | | |
|---|---|---|
| **sulfinic acids** | | |
| p-Toluene- | 1.99 | 73 |
| p-Chlorobenzene- | 73 | |
| p-Nitrobenzene- | 73 | |
| p-Bromobenzene- | 1.89 | 73 |
| m-Nitrobenzene- | 1.88 | 73 |
| Benzene- | 1.84, 2.16 | 73 |

| **Peroxyacids** | | |
|---|---|---|
| Peroxymonosulfuric | 9.4 | 69 |
| Acetic | 8.2 | 70 |
| n-Butyric | 8.2 | 70 |
| Formic | 7.1 | 70 |
| Propionic | 8.1 | 70 |
| peroxydiphosphoric | 5.18, 7.8 | 85 |
| peroxymonophosphoric | 4.85 | 90 |

| | |
|---|---|
| 4-Pyridine-1,2-ethanedione-2-oxime methiodide | 7.1 |
| Pyridine-2-aldoxime methiodide | 8.0 |
| Phenylglyoxald- | 8.3 |
| Pyridine-4-aldoxime dodeciodide | 8.5 |
| Pyridine-3-alkoxime methiodide | 9.2 |

| **Hydroxamic acids** | ref. 93 |
|---|---|
| D-Lysine- | 7.93 |
| N-phenylnicotino- | 8.00 |
| Chloroaceto- | 8.40 |
| Formo- | 8.65 |
| p-Chlorophenoxyaceto- | 8.75 |
| p-Hydroxybenzo- | 8.93 |
| p-Methoxybenzo- | 9.00 |
| N-Phenylbenzo- | 9.15 |
| o-Aminobenzo- | 9.17 |
| L-Tyrosine | 9.20 |
| L-Lysine | 7.9 |
| p-Nitrobenzo- | 8.0 |
| p-Aminobenzo- | 9.3 |
| L-Lacti- | 9.3 |
| Propiono- | 9.4 |
| Phthalo- | 9.4 |
| Indole-3-aceto- | 9.5 |
| Cyclohexano- | 9.7 |
| Hexano- | 9.7 |

**Amino Acids**

| **Compound** | **pK -COOH** | **-$NH_3$** | **Ref.** |
|---|---|---|---|
| Alanine | 2.35 | 9.69 | 6 |
| α-Aminobutyric acid | 2.55 | 9.60 | |
| α-Aminoisobutyric | 2.36 | 10.21 | 6 |
| Argininosuccinic | >12, 1.62 2.70, 4.26 | 9.58 | 6 |
| Aspartic acid | 2.09, 3.86 | 9.82 | 6 |
| Canaline | 10.3, 9.20 | 11.6 (?) | 6 |
| Creatinine | 4.84 | 9.2 | 6 |
| Cystine | 1.65 | 7.85 | 6 |
| | 2.26 | 9.85 | 6 |
| Diidotyrosine | 6.48, 2.12 | 7.82 | 6 |
| Glutamic acid | 2.19, 4.25 | 9.67 | 6 |
| Glycine | 2.34 | 9.6 | 6 |
| Histidine | 6.0, 1.82 6 | | 9.17 |
| Hydroxylsine | 2.13 | 8.62 9.67 | 6 |
| Isoleucine | 2.36 | 9.68 | 6 |
| Lysine | 2.18 | 8.95 10.53 | 6 |
| O-Methyl tyrosine | | 9.27 | 21 |
| O-Methyltyrosine ethyl ester | 7.31 | | 22 |
| octopine | 13, 1.36 6 2.40 | | 8.77 |
| Phenylalanine | 1.83 | 9.13 | 6 |
| 2-Pyrrolidoone-5-carboxylic acid (glucamic acid) | 3.32 | | |
| Serine | 2.21 | 9.15 | 6 |
| Threonine | 2.63 | 10.43 | 6 |
| N-Trimethyl tyrosine | | 9.75 | 21 |
| Tyrosine | 10.07, 2.20 | 9.11 | |
| Urocanic acid | 5.8 | 3.5 | |
| Valine | 2.32 | 9.62 | 6 |
| β-Alanine | 3.60 | 10.19 | 6 |
| γ-Aminobutyric acid | 4.23 | 10.43 | 6 |
| Arginine 12.48 | 2.17 | 9.04 | 6 |
| Asparagine | 2.02 | 8.8 | 6 |
| Azaserine | 8.55 | | 6 |
| Canavanine | 7.40, 9.25 | 11.50 (?) | 6 |
| Creatine | 2.67 | 11.02 | 6 |
| Cysteine 10.78 | 1.71 | 8.33 | 6 |
| 3,4-Dihydroxyphenylalanine | 9.88, 2.36 11.68 | 8.68 | 6 |
| Glutamine | 2.17 | 9.13 | 6 |
| Histamine 5.0 | | 9.7 | 6 |
| β-Hydroxyglutamic acid | 2.09 4.18 | 9.20 | 6 |
| Hydroxyproline | 1.92 | 9.73 | 6 |
| Leucine | 2.36 | 9.60 | 6 |
| Methionine | 2.28 | 9.21 | |
| 1-Methylhistidine | 6.48, 1.69 | 8.85 | 6 |
| Norleucine | 2.39 | 9.76 | 6 |
| Norvaline | 2.36 | 9.76 | 6 |
| Ornithine | 1.71 | 8.69 10.76 | 6 |
| Proline | 1.99 | 10.60 | 6 |
| Sarcosine | 2.23 | 10.01 | 6 |
| Taurine 1.5 | | 8.74 | 6 |
| Thiolhistidine <1.5, 11.4 | 1.84 | 8.47 | 6 |
| Tryptophan | 2.38 | 9.39 | 6 |
| Tyrosine ethyl ester | 7.33 | 9.80 | 22 |
| **Peptides** | | | |
| Anserine 7.0 | 2.65 | 9.5 | 6 |
| Carnosine 6.83 | -- | 9.51 | 6 |
| Cystinyldiglycine | 3.12 3.12 | 6.36 6.95 | 6 |
| Glycylglycine | 3.06 | 8.13 | |
| Gly-gly-gly | 3.26 | 7.91 | 23 |
| Glycylproline | 2.84 | 8.55 | 6 |
| Aspartyl histi- | 2.45 | 7.98 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| dine | 6.82 | 3.02 | | Gly-gly-gly-gly | 3.05 | 7.75 | 23 |
| Diglycylcystine | 2.71 | 7.94 | 6 | Lysyl-lysine (L,L) | 3.01 | 7.53 | 6 |
| Glutathione 9.12 | 2.12 | 8.66 | 6 | | 10.05 | 11.01 | |
| | 3.53 | | | | | | |

| **Compound** | **-COOH** | **α-$NH_2$** | **ε-$NH_2$** | **ε-$NH_2$** | **ε-$NH_2$** | **Ref.** |
|---|---|---|---|---|---|---|
| Gly•Ala (L) or (D) | 3.17 | 8.23 | | | | 27 |
| Ala•Gly (L) or (D) | 3.16 | 8.24 | | | | 27 |
| Gly•Ala•Ala (LL) | 3.38 | 8.10 | | | | 27 |
| Gly•Ala•Ala (LD) | 3.30 | 8.17 | | | | 27 |
| Ala•Ala•OH (DD) | 3.30 | 8.14 | | | | 27 |
| Ala•Ala•OH (LD) | 3.12 | 8.30 | | | | 27 |
| H•Ala•Ala•Ala•OH (3L) | 3.39 | 8.03 | | | | 27 |
| H•Ala•Ala•Ala•OH (LLD) | 3.37 | 8.05 | | | | 27 |
| H•Ala-Ala-Ala•OH (LDL) | 3.31 | 8.13 | | | | 27 |
| H•Ala-Ala-Ala•OH (DLL) | 3.37 | 8.06 | | | | 27 |
| H-Ala-Ala-Ala•OH (3D) | 3.39 | 8.06 | | | | 27 |
| H•Ala-Ala-Ala-Ala•OH (4L) | 3.42 | 7.94 | | | | 27 |
| H•Ala-Ala-Ala-Ala•OH (LLDL) | 3.24 | 7.93 | | | | 27 |
| H•Ala-Ala-Ala-Ala•OH (LDLL) | 3.22 | 7.99 | | | | 27 |
| H•Ala-Ala-Ala-Ala•OH (DLLL) | 3.42 | 7.99 | | | | 27 |
| H•Lys-Ala•OH (LL) | 3.22 | 7.62 | 10.70 | | | 27 |
| H•Lys-Ala•OH (LD) | 3.00 | 7.74 | 10.63 | | | 27 |
| H•Ala-Lys-Ala•OH (3L) | 3.15 | 7.65 | 10.30 | | | 27 |
| H•Ala-Lys-Ala•OH (LDL) | 3.33 | 7.97 | 10.36 | | | 27 |
| H•Ala-Lys-Ala•OH (LLD) | 3.29 | 7.84 | 10.49 | | | 27 |
| H•Ala-Lys-Ala-Ala•OH (4L) | 3.58 | 8.01 | 10.58 | | | 27 |
| H•Ala-Lys-Ala•OH (LDLL) | 3.32 | 8.01 | 10.37 | | | 27 |
| H•Ala-Lys-Ala-Ala-Ala•OH (5L) | 3.53 | 7.75 | 10.35 | | | 27 |
| H•Ala-Lys-Ala-Ala-Ala•OH (LDLLL) | 3.30 | 7.85 | 10.29 | | | 27 |
| H•Lys-Lys•OH (LL) | 3.01 | 7.53 | 10.05 | 11.01 | | 27 |
| H•Lys-Lys•OH (LD) | 2.85 | 7.53 | 9.92 | 10.98 | | 27 |
| H•Lys-Lys•OH (3L) | 3.08 | 7.34 | 9.80 | 10.54 | 11.32 | 27 |
| H•Lys-Lys-Lys•OH (LDL) | 2.91 | 7.29 | 9.79 | 10.54 | 11.42 | 27 |
| H•Lys-Lys-Lys•OH (LDD) | 2.94 | 7.14 | 9.60 | 10.38 | 11.09 | 27 |

| **Compound** | **pK** | | | **ref.** |
|---|---|---|---|---|
| Glutathione | 3.59, 8.75, 9.65 | | | 77 |
| Glycylserine | 8.23 | | | 77 |
| Glycylleucine | 8.13 | | | 77 |
| Leucylglycine | 7.96 | | | 77 |
| Glycylisoleucine | 7.96 | | | 77 |
| Leucylglycylglycine | 7.66 | | | 77 |
| Glycylphenylalanine | 8.28 | | | 77 |
| Glycyltyrosine | 8.22 | | | 77 |
| Benzylglutamic acid | 3.49, 4.99 | | | 77 |
| Glycyltryptophane | 8.04 | | | 77 |
| Glutathione, oxidized | 3.15, 4.03, 8.57, 9.54 | | | 77 |
| Alanylalanine (LL) | 3.30 | 8.14 | | 92 |
| Alanylalanine (LD) | 3.12 | 8.30 | | 92 |
| Lysylalanine (LL) | 3.22 | 7.62 | 10.70 | 92 |
| Lysylalanine (LD) | 3.00 | 7.74 | 10.63 | 92 |
| Leucyltyrosine (LL) | 3.46 | 7.84 | 10.09 | 92 |
| Leucyltyrosine (DL) | 3.12 | 8.38 | 10.35 | 92 |

| | | | | |
|---|---|---|---|---|
| Lysyllysine (LD) | 2.85 | 7.53 | 9.92 | 92 |

**NITROGEN COMPOUNDS**

| **Aliphatic Amines** | **pK** | **ref.** | | | |
|---|---|---|---|---|---|
| Ammonia | 9.21 | 1 | n-Propyl- | 10.53 | 1 |
| Primary Amines | | | Trimethylsilymethyl- | 10.96 | 1 |
| β-Alanine ester | 9.13 | 1 | $CH_3ONH_2$ | 4.60 | 12 |
| Allylamine- | 9.69 | 2 | Allyl- | 9.49 | 1 |
| Benzyl | 9.34 | 1 | γ-Amino-n-butyric acid ester | 9.71 | 1 |
| n-Butyl- | 10.59 | 1 | sec-Butyl- | 10.56 | 1 |
| t-Butyl- | 10.55 | 1 | Cyclohexyl- | 10.64 | 1 |
| Cyclohexylmethyl- | 10.49 | 1 | β-difluoroethyl- | 7.52 | 1 |
| Ethanol- | 9.50 | 1 | Ethyl | 10.63 | 1 |
| Ethylenedi- | 9.98, 7.52 | 1, 77 | Glycine ester | 7.75 | 1 |
| Hydrazine | 8.10 | 1 | Hydroxyl- | 5.97 | 1 |
| Isopropyl- | 10.63 | 1 | Methoxy- | 4.60 | 1 |
| Methyl- | 10.62 | 1 | neo-Pentyl- | 10.21 | 1 |
| Phenylamyl- | 10.49 | 2 | δ-Phenylbutyl | 10.40 | 2 |
| β-Phenylethyl- | 9.83 | 1 | γ-Phenylpropyl- | 10.20 | 1 |
| | | | Triethylenedi- | 8.8* | ? |

| **X** | **$XNH_3^+$** | **$XCH_2NH_3^+$** | **$X(CH_2)_2NH_3^+$** | **$X(CH_2)_3NH_3^+$** | **$X(CH_2)_4NH_3^+$** | **$X(CH_2)_5NH_3^+$** | **ref.** |
|---|---|---|---|---|---|---|---|
| H- | 9.25* | 10.64* | 10.67* | 10.58* | 10.61* | 10.63* | 2 |
| $HF_2C$- | | 7.52 | | | | | |
| $RO_2C$- | | 7.75 | 9.13 | 9.71 | 10.15* | 10.37 | 2 |
| HO- | 5.96* | | 9.50* | | | | |
| $C_6H_5$- | 4.58* | 9.37* | 9.83* | 10.20* | 10.39* | 10.49* | 2 |
| $H_2N$- | 8.12* | | 9.98* | 10.65* | 10.84* | 11.05* | 2 |
| $H_2C$=CH- | | 9.69 | | | | | |
| $CH_3$- | 10.64* | 10.67* | 10.58* | 10.61* | 10.63* | 10.64* | 2 |

| **X** | **-H** | **$-NH_3^+$** | **$-CO_2^-$** | **$-SO_3^-$** | **$-PO_3^-$** | 2 |
|---|---|---|---|---|---|---|
| $X\text{-}NH_3^+$ | 9.25* | -.88 | | 1 | 10.25 | |
| $X(CH_2)_2NH_3^+$ | 10.64 | | 9.77 | 5.75 | 10.8 | |
| $X(CH_2)_2NH_3^+$ | 10.67 | | 10.19 | 9.20 | 10.8 | |
| $X(CH_2)_4NH_3^+$ | 10.61 | 9.31 | 10.77 | 10.65 | 10.9 | |
| $X(CH_2)_5NH_3^+$ | 10.63 | 9.74 | 10.75 | 10.95 | 11.0 | |
| $X(CH_2)_8NH_3^+$ | 10.65 | 10.10 | | | | |
| $X(CH_2)_{10}NH_3^+$ | 10.64 | | | 11.35 | 11.25 | |
| $X(CH_2)_3NH_3^+$ | 10.58 | 8.59 | 10.43 | 10.05 | | |

| **Secondary amines** | | | | | |
|---|---|---|---|---|---|
| Dimethyl- | 10.64 | 1 | Di-n-butyl- | 11.25 | 1 |
| Di-n-propyl- | 11.00 | 1 | Diisobutyl- | 10.50 | 1 |
| Diisopropyl- | 11.05 | 1 | α-Ethylpyrroline | 7.43 | 2 |
| t-Butylcyclohexyl- | 11.23 | 1 | α-Benzylpyrroline- | 7.08 | 2 |
| α-Cyclohexylpyrroline | 7.95 | 2 | 2-Methylpiperidine | 10.99 | 2 |
| α-(p-Tolyl)pyrroline | 7.59 | 2 | α-Cyclohexylpyrrolidine | 10.80 | 2 |
| α-Ethylpyrrolidine | 10.43 | 2 | α-(p-Tolyl)pyrrolidine | 10.01 | 2 |
| α-Benzylpyrrolidine | 10.36 | 2 | N,O-dimethylhydroxylamine | 4.75 | 12 |
| N-methylhydroxylamine | 5.96 | 12 | Acetanilide | +0.61 | 4 |
| Diethyl- | 10.98 | 1 | **thermodynamic value* | | |

**Aliphatic Amines**

| | | |
|---|---|---|
| 1,2-Iminoethane | 7.98 | 7 |
| cis-2,3-Iminobutane | 8.72 | 7 |
| 1,2-Imino-2-methylpropane | 8.61 | 7 |
| 1,2-Iminobutane | 8.29 | 7 |
| trans-2,3-Iminobutane | 8.69 | 7 |

**Secondary Amines**

| | | |
|---|---|---|
| Allylmethyl- | 10.11 | 1 |
| Benzylethyl- | 9.68 | 1 |
| Morpholine | 8.36 | 1 |
| N-Benzoylpiperazine | 7.78 | 1 |
| Di-sec-butyl- | 11.01 | 1 |
| N-Methylmethoxyamine | 4.75 | 1 |
| Pyrolidine | 11.27 | 1 |
| 1-Tosylpiperazine | 7.39 | |
| Benzylmethyl- | 9.58 | 1 |
| Piperidine | 11.22 | 1 |
| N-Carbethoxypiperazin | 8.28 | 1 |
| Dietrimethylsilylmethyl- | 11.40 | 1 |
| Diallyl- | 9.29 | 1 |
| N-Methylhydroxyl- | 5.96 | 1 |
| Trimethyleneimine | 11.29 | 1 |
| Cis-2,6-dimethyl-piperidine | 10.92 | 3 |

**Tertiary amines**

| | | |
|---|---|---|
| Trimethyl- | 9.76 | 1 |
| Dimethyldiethyl- | 10.29 | 1 |
| Dimethyl-n-propyl- | 9.99 | 1 |
| Dimethyl-isobutyl- | 9.91 | 1 |
| Dimethyl-sec-butyl- | 10.40 | 1 |
| Tri-n-propyl- | 10.65 | 1 |
| Triallyl- | 8.31 | 1 |
| N-Allylpiperidine | 9.69 | 2 |
| 1-Diethylamino-hexane-thiol-(6) | | |

**Cyanoamines**

| | | |
|---|---|---|
| N-piperidine-$CH_2CN$ | 4.55 | 8 |
| $Et_2NCN$ | -2.0 | 8 |
| $Et_2N(CH_2)_2CN$ | 7.65 | 8 |
| $Et_2N(CH_2)_4CN$ | 10.08 | 8 |
| $Et_2NC(CH_3)_2CN$ | 9.13 | 8 |
| $EtN(CH_2CN)_2$ | -0.6 | 8 |
| $EtN(CH_2CH_2CN)_2$ | 4.55 | 8 |
| $H_2NCH_2CN$ | 5.34 | 8 |
| N-Amphetamine-$(CH_2)_2$-CN | 7.23 | 8 |
| N-Norcodeine-$(CH_2)_2CN$ | 5.68 | 8 |
| Dimethylcyanimide | 1.2 | 9 |
| Diethylcyanimide | 1.2 | 9 |
| Aminoacetonitrile | 5.3 | 9 |
| Diethylaminoacetonitrile | 4.5 | 9 |

| | | |
|---|---|---|
| Methyl-β-diethylamino-ethyl-sulfide | | |
| 1,2-Dimethyl-$\Delta^2$-pyrroline | 11.94 | 2 |
| 1-methyl-2-n-butyl-$\Delta^2$-pyrroline | 11.90 | |
| 1-Ethyl-2-methyl-$\Delta^2$-pyrroline | 11.92 | 2 |
| 1-n-Butyl-2-methyl-$\Delta^2$-pyrroline | 11.90 | 2 |
| 1,2-Dimethyl-$\Delta^2$-tetrahydropyridine | 11.57 | 2 |
| N-Ethyl derivative of: 1,2-Imino-ethane | 7.93 | 7 |
| Trans-2,3-Iminobutane | 9.47 | 7 |
| Trimethylhydroxylamine | 3.65 | 12 |
| Dimethylethyl- | 9.99 | 1 |
| Triethyl- | 10.65 | 1 |
| Dimethyl-n-butyl- | 10.02 | 1 |
| Dimethyl-isopropyl- | 10.30 | 1 |
| Dimethyl-t-butyl- | 10.52 | 1 |
| Tri-n-butyl- | 10.89 | 1 |
| Diallylmethyl- | 8.79 | 1 |
| 1-n-Propylpiperidine | 10.48 | 2 |
| 10.1 | 10.1 | 5 |
| 9.8 | -- | 5 |
| 1,2-Dimethylpyrrolidine | 10.26 | 2 |
| 1-Methyl-2-n-butylpyrrolidin | 10.24 | 2 |
| 1-Ethyl-2-methylpyrrolidine | 10.64 | 2 |
| 1-n-Butyl-2-methylpyrrolidine | 10.43 | 2 |
| 1-Ethyl-2-methylpyrrolidine | 10.70 | 2 |
| 1,2-Iminobutane | 8.18 | 7 |
| cis-2,3-Iminobutane | 8.56 | 7 |
| N-dimethylhydroxylamine | 5.20 | 12 |
| Allyldimethyl | 8.78 | 1 |
| 1,2-Dimethylpiperidine | 10.26 | 2 |
| 1-Ethyl-2-methyl-$\Delta^2$-tetrahydropyridine | 11.57 | 2 |

| | | |
|---|---|---|
| 2-Amino-2-cyanopropane | 5.3 | 9 |
| β-Isopropylaminopropionitrile | 8.0 | 9 |
| β-Diethylaminopropionitrile | 7.6 | 9 |
| $Et_2NCH_2CN$ | 4.55 | 8 |
| $Et_2N(CH_2)_3CN$ | 9.29 | 8 |
| $Et_2N(CH_2)_5CN$ | 10.46 | 8 |
| $HN(CH_2CN)_2$ | 0.2 | 8 |
| $HN(CH_2CH_2CN)_2$ | 5.26 | 8 |
| $N(CH_2CH_2CN)_3$ | 1.1 | 8 |
| N-piperidine-$C(CH_3)_2CN$ | 9.22 | 8 |
| N-Methamphetamine-$(CH_2)_2CN$ | 6.95 | 8 |
| Methyl cyanamide | 1.2 | 9 |
| Ethyl cyanamide | 1.2 | 9 |
| Cyanamide | 1.1 | 9 |
| Dimethylaminoacetonitrile | 4.2 | 9 |

| | | |
|---|---|---|
| β-Aminopropionitrile | 7.7 | 9 |
| β-Dimethylaminopropionitrile | 7.0 | 9 |
| β,β"-Dicyanodiethylamine | 5.2 | 9 |

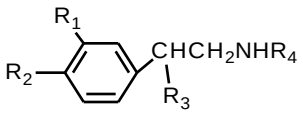
*For complex chelating agents of aliphatic amines, see also ref. 77.*

**Fluoro-substituted amines**

| | | |
|---|---|---|
| $CF_3CH_2NH_2$ | 5.7 | 10 |
| $CF_3CH_2N(CH_3)_2$ | 4.75 | 10 |
| $CF_3CH_2NHCH_3$ | 6.05 | 10 |

**Phenylethylamines**

| | | |
|---|---|---|
| 2-phenylethylamine | 9.78 | 11 |
| N-methyl-2-(3,4-dihydroxyphenyl)-ethylamine | 8.78 | 11 |
| N-methyl-2-phenyl | 10.31 | 11 |
| Epinephrine | 8.55 | 11 |
| Arterenol | 8.55 | 11 |




ref. 11

| $R_1$ | $R_2$ | $R_3$ | $R_4$ | pK |
|---|---|---|---|---|
| H | H | H | H | 9.78 |
| H | H | OH | H | 8.90 |
| H | OH | OH | H | 8.81 |
| OH | H | OH | H | 8.67 |
| H | OH | H | H | 9.22 |
| OH | OH | H | H | 8.93 |
| OH | OH | OH | H | 8.58 |
| H | H | H | $CH_3$ | 10.31 |
| H | H | OH | $CH_3$ | 9.31 |
| H | OH | OH | $CH_2$ | 8.62 |
| OH | H | OH | $CH_3$ | 8.89 |
| H | OH | H | $CH_3$ | 9.36 |
| OH | OH | H | $CH_3$ | 8.78 |
| OH | OH | OH | $CH_3$ | 8.55 |

**Ring amines and imines** (in 80% methyl cellosolve) (ref. 2)

| | |
|---|---|
| Pentamethylene | 9.99 |
| Hexamethylene | 10.00 |
| Heptamethylene | 9.77 |
| Octamethylene | 9.39 |
| Nonamethylene | 9.14 |
| Decamethylene | 9.04 |
| Undecamethylene | 9.14 |
| Dodecamethylene | 9.31 |
| Tridecamethylene | 9.35 |
| Tetradecamethylene | 9.35 |
| Hexadecamethylene | 9.29 |
| Heptadecamethylene | 9.27 |
| Cyclohexyl | 9.82 |
| Cycloheptyl | 9.99 |
| Cyclooctyl | |
| Cyclononyl | 9.95 |
| Cyclodecyl | 9.85 |
| Cycloundecyl | 9.71 |
| Cyclododecyl | 9.62 |
| Cyclotridecyl | 9.63 |
| Cyclotetradecyl | 9.54 |
| Cyclopentadecyl | 9.54 |
| Cycloheptadecyl | 9.57 |
| Cyclooctadecyl | 9.54 |

**Amines other**

| | | |
|---|---|---|
| Dimeoone | 5.23 | 18 |
| Phthalimide | 8.30 | 18 |
| Nitrourea | 4.57 | 18 |
| Nitrourethane | 3.28 | 18 |
| Diphenylthiocarbazone | 4.5 | 6 |
| β,β,β"-Triaminotriethylamine | 8.42, 9.44, 10.13 | 87 |

**Anilines** Ref. 2

**Monosubstituted**

| **Substituent** | **o** | **m** | **p** |
|---|---|---|---|
| H- | 4.62* | 4.64* | 4.58* |

| | | | |
|---|---|---|---|
| $(CH_3)_3N^+$- | | 2.26 | 2.51 |
| $CH_3O_2C$- | 2.16 | 3.56 | 2.30 |
| $CH_3SO_2$- | | 2.68* | 1.48 |
| $CH_3S$- | | 4.05 | 4.40 |
| Br- | 2.60* | 3.51* | 3.91* |
| F- | 2.96* | 3.38* | 4.52* |
| $CH_3O$- | 4.49* | 4.20* | 5.29* |
| $C_6H_5$- | 3.78* | 4.18 | 4.27* |
| $(CH_3)_3C$- | 3.78 | | |
| $^-O_3S$- | | 3.80 | 3.32 |
| $H_3N^+$ | 1.3 | 2.65 | 3.29 |
| $O_2N$- | -0.28* | 2.45* | 0.98*, 1.11* |
| $HO_2C$- | 2.04 | 3.05 | 2.32 |
| $C_2H_5O_2C$- | 2.10 | | 2.38 |
| $F_3C$- | | 3.49* | 2.57* |
| HO- | 4.72 | 4.17 | 5.50 |
| Cl- | 2.62* | 3.32* | 3.81* |
| $(CH_3)_3Si$- | | 4.64* | 4.36* |
| $C_2H_5O$- | 4.47* | 4.17* | 5.25* |
| $CH_3$- | 4.38* | 4.67* | 5.07* |
| $^-HO_3As$ | 3.77 | 4.05 | 4.05 |
| $H_2N$- | 4.47 | 4.88 | 6.08 |

**Thermodynamic*

| | | | |
|---|---|---|---|
| p-$(CH_3)_3C$- | 4.65 | | |
| m-Br- | 3.08 | | |
| m-Cl- | 3.09 | | |
| p-F- | 4.01 | | |
| p-$(CH_3)_3Si$- | 3.99 | | |
| p-$CH_3O$- | 5.14, 5.16 | | |

**Dimethyl**

| | | |
|---|---|---|
| H | 5.07 | 52 |
| m-$NO_2$ | 2.63 | 52 |
| m-CN | 2.97 | 52 |
| p-$NO_2$ | 0.61 | 52 |
| p-CN | 1.78 | 52 |
| p-NO | 4.54 | 52 |

**Dimethyl** (in 50% ethanol)

| **Substituent $XC_6H_4N(CH_3)_2$** | ref. 2 |
|---|---|
| H- | 4.21, 4.09 |
| m-$CH_3$ | 4.66 |
| p-$C_2H_5$- | 4.69 |
| o-$(CH_3)_2CH$- | 5.05 |
| p-$CH_3CH_2CH_2CH_2$- | 4.62 |
| o-$(CH_3)_3C$- | 4.26 |
| p-I- | 3.43, 2.73 |
| p-Br- | 3.52, 2.82 |
| p-Cl- | 3.33 |
| m-$(CH_3)_3Si$- | 4.41 |
| o-$CH_3O$- | 5.49 |
| o-$CH_3$ | 5.15, 5.07 |
| p-$CH_3$ | 4.94 |
| p-$CH_3CH_2CH_2$- | 4.43 |
| p-$(CH_3)_2CH$- | 4.77 |
| p-$(CH_3)_2CHCH_2$- | 4.19 |

**Ortho-substituted anilines** (in 50% ethanol)

| | |
|---|---|
| H- | 4.25 |
| 2-$CH_3$- | 3.98, 4.09 |
| 2,3-$(CH_3)_2$- | 4.42 |
| 2,4-$(CH_3)_2$- | 4.61 |
| 2,5-$(CH_3)_2$- | 4.17, 4.23 |
| 2,6-$(CH_3)_2$- | 3.42, 3.49 |
| 3,5-$(CH_3)_2$- | 4.48 |
| 2-$CH_3$- | 4.09 |
| 2-$(CH_3)_2CH$- | 4.06 |
| 2-$(CH_3)_2C$- | 3.38 |
| 2,6-$(CH_3)_2$-4-$(CH_3)_3C$- | 3.88 |
| 2,4-$(CH_3)_2$-6-$(CH_3)_3$- | 3.43 |
| 2-$CH_3$-4,6-$(CH_3)_3C$- | 3.31 |
| 2,4,6-[$(CH_3)_3C_3$]- | <2 |

**Substituted Naphthylamines**

| | |
|---|---|
| 1-$NH_2$- | 3.92* |
| 1-$NH_2$-2-$NO_2$- | -1.6 |
| 1-$NH_2$-3-$NO_2$- | 2.22 |
| 1-$NH_2$-4-$NO_2$- | 0.54 |
| 1-$NH_2$-5-$NO_2$- | 2.80 |
| 1-$NH_2$-6-$NO_2$- | 3.15 |
| 1-$NH_2$-7-$NO_2$- | 2.83 |
| 1-$NH_2$-8-$NO_2$- | 2.79 |
| 1-$NH_2$-8-$SO_3$- | 1.71 |
| 1-$NH_2$-3-$SO_3$- | 3.20* |
| 1-$NH_2$-4-$SO_3$- | 2.81* |
| 1-$NH_2$-5-$SO_3$- | 3.69* |
| 1-$NH_2$-6-$SO_3$- | 3.80* |
| 1-$NH_2$-7-$SO_3$- | 3.66 |
| 1-$NH_2$-8-$SO_3$- | 5.03* |
| 2-$NH_2$- | 4.11* |
| 2-$NH_2$-1-$NO_2$- | -1.0 |
| 2-$NH_2$-3-$NO_2$- | 2.93 |
| 2-$NH_2$-4-$NO_2$- | 2.63 |
| 2-$NH_2$-5-$NO_2$- | 3.16 |
| 2-$NH_2$-6-$NO_2$- | 2.75 |
| 2-$NH_2$-7-$NO_2$- | 3.13 |
| 2-$NH_2$-8-$NO_2$- | 2.86 |
| 2-$NH_2$-1-$SO_3$- | 2.35 |
| 2-$NH_2$-3-$SO_3$- | -- |
| 2-$NH_2$-4-$SO_3$- | 3.70 |
| 2-$NH_2$-5-$SO_3$- | 3.96* |
| 2-$NH_2$-6-$SO_3$- | 3.74* |
| 2-$NH_2$-7-$SO_3$- | 3.95* |
| 2-$NH_2$-8-$SO_3$- | 3.89* |

**N-substituted anilines***

| R | $C_6H_5NHR$ | $C_6H_5N(CH_3)R$ | $C_6H_5NR_2$ | 2-$CH_3C_6H_4NHR$ | 2-$CH_3C_6H_4NR_2$ |
|---|---|---|---|---|---|
| H- | 4.58 | 4.85 | 4.58 | 4.39 | 4.39 |
| $CH_3$- | 4.85 | 5.06 | 5.06 | 4.59 | 5.86 |
| $C_2H_5$- | 5.11 | 5.98 | 6.56 | 4.92 | 7.18 |
| n-$C_3H_7$- | 5.02 | -- | 5.59 | -- | |
| n-$C_4H_9$- | 4.95 | -- | ~5.7 | -- | |
| i-$C_4H_9$- | -- | 5.20 | -- | -- | |
| sec-$C_4H_9$- | -- | 6.04 | -- | -- | |
| t-$C_6H_{12}$- | 6.30 | -- | -- | -- | |
| Cyclopentyl- | 5.30 | 6.71 | -- | 5.07 | |
| Cyclohexyl- | 5.60 | 6.35 | -- | 5.34 | |
| t-$C_4H_9$- | 6.95 | 7.52 | -- | 6.49 | |

**Thermodynamic*

**AMINES** ref. 77

**Primary amines**

| | |
|---|---|
| 2-aminoethylsulphonic acid | 9.08 |
| Aminomalonic acid | 3.32, 9.83 |
| N-n-butylethylenediamine | 7.53, 10.30 |
| 2,3-diaminobutane, meso | 6.92, 9.97 |
| 2,3-diaminobutane, racemic | 6.91, 10.00 |
| 2,2'-diaminodiethyl sulfide | 8.84, 9.64 |
| 1,3-diamino-2,2-dimethylpropane | 8.18, 10.22 |
| N,N'-Di-(2-aminoethyl)-ethylenediamine | 3.32, 6.67, 9.20, 9.92 |
| 1,2-diamino-2-methylpropane | 6.79, 10.00 |
| 1,3-Diaminopropan-2-ol | 8.23, 9.68 |
| N,N'-Diglycyethylenediamine | 7.63, 8.35 |
| Ethylenediamine-N,N-diacetic acid | 5.58, 11.05 |
| Furfurylamine | 8.89 |
| 2-(2-hydroxypropylamino)-ethylamine | 6.94, 9.86 |
| 2-(3-hydroxypropylamino)ethylamine | 6.78, 9.76 |
| N-Methylaminoacetic acid | 2.24, 10.01 |
| Methyl-α-amino-β-mercaptoproionate | 6.56, 8.99 |
| N-n-propylethylenediamine | 7.54, 10.34 |
| 1,2,3-triaminopropane | 3.72, 7.95, 9.59 |
| Tris-(hydroxymethyl)-aminomethane | 8.10 |
| 2-amino-2'-hydroxydiethyl sulfide | 9.04 |
| N-(carbamoylmethyl)-iminodiacetic acid | 2.30, 6.60 |
| 2,2'-diaminodiethylamine | 3.58, 8.86, 9.65 |
| 2,3-diamino-2,3-dimethylbutane | 6.56, 10.13 |
| 3,3'-diaminodi-n-propylamine | 8.02,9.70, 10.7 |
| 1,2-Di-(2-aminoethylthio)ethane | 8.43, 9.32 |
| 1,2-diaminopropane | 7.13, 10.00 |
| N,N-diethylethylenediamine | 7.07, 10.02 |
| N,N-dimethylethylenediamine | 6.63, 9.53 |
| N-Ethylethylenediamine | 7.63, 10.56 |
| N-(2-hydroxyethyl)-ethylenediamine | 6.83, 9.82 |
| N-isopropylethylenediamine | 7.70, 10.62 |
| 2-Methoxyethylamine | 9.20 |
| Mercaptoethylamine | 8.27, 10.53 |
| N-Methylethylenediamine | 7.56, 10.40 |
| 2-Methylthioethylamine | 9.18 |
| 2-thienylmethylamine | 8.92 |
| Triaminotriethylamine | 8.56, 9.59, 10.29 |

**Secondary amines**

| | |
|---|---|
| N-Butylaminoacetic acid | 2.29, 10.07 |
| N,N'-Diethylethylenediamine | 7.70, 10.46 |
| 2,2'-dihydroxydiethylamine | 9.00 |
| N,N'-di-n-propylethylenediamine | 8.14, 10.97 |
| Ethylenediamine-N,N'-diacetic acid | 6.42, 9.46 |
| Iminodipropionic acid | 4.11, 9.61 |
| Piperazine | 5.68, 9.82 |
| β-carboxymethylaminopropionic acid | 3.61, 9.46 |
| N,N'-Dimethylethylenediamine | 7.40, 10.16 |
| N-ethylaminoacetic acid | 2.30, 10.10 |
| Iminodiacetic acid | 2.98, 9.89 |
| N-isopropylaminoacetic acid | 2.36, 10.06 |
| N-n-propylaminoacetic acid | 2.28, 10.03 |

**Tertiary amines**

| | |
|---|---|
| 4-(2-aminoethyl)morpholine | 4.84, 9.45 |
| Di-(2-hydroxyethyl)aminoacetic acid | 8.08 |
| Hexamethylenetetramine | 5.13 |
| Methyliminodiacetic acid | 2.81, 10.18 |
| Diethylaminoacetic acid | 2.04, 10.47 |
| Dimethylaminoacetic acid | 2.08, 9.80 |
| N-2-hydroxyethyliminodiacetic acid | 2.2, 8.73 |
| Triethylenediamine | 4.18, 8.19 |

**Ref. 1**

| | |
|---|---|
| Diallylmethyl | 8.79 |
| Benzyldimethyl | 8.93 |
| N-Allylpiperidine | 9.68 |
| N-Allylmorpholine | 7.05 |
| Propargyldimethyl | 7.05 |
| Propargylethyldimethyl | 8.88 |
| N-Methylmorpholine | 7.41 |
| N-Methylpyrrolidine | 10.46 |
| N,N-Dimethylhydroxylamine | 5.20 |
| Allyldimethyl | 8.73 |
| Benzyldiethyl | 9.48 |
| N-Ethylpiperidine | 10.40 |
| N-Ethylmorpholine | 7.70 |
| Propargymethyldimethyl | 8.33 |
| N-Methylpiperidine | 10.08 |
| N-Methyltrimethyleneimine | 10.40 |
| Triethanolamine | 7.77 |
| N,N-Dimethylmethoxyamine | 3.65 |

**Ref. 5**

| | |
|---|---|
| N-Dimethyl-cysteamine | 7.95, 10.7 |
| N-Dipropyl-cysteamine | 8.00, 10.8 |
| N-β-Mercaptoethyl-morpholine | 6.65, 9.8 |
| 1-Diethylamino-butan- (4) | 10.1 |
| Methyl-[β-diethylamino-ethyl]sulfide | 9.8 |
| N-Diethyl-cysteamine | 7.8, 10.75 |
| N-β-Mercaptoethyl-piperidine | 7.95, 11.05 |
| 1-Diethylamino-propan- (3) | 8.0, 10.5 |
| 1-Diethylamino-hexan- (6) | 10.1 |

**ANILINES** (Ref. 88)

**m-Substituted anilines**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| m-$C_2H_5$ | 4.70 | | | m-$CH(CH_3)_2$ | 4.67 | | |
| -$C(CH_3)_3$ | | 4.66 | | 3,5-$(CH_3)_2$ | | 4.74 | |
| 3,5-$[C(CH_3)_3]_2$ | 4.97 | | | m-$COCH_3$ | 3.56 | | |
| m-CN | 2.76 | | | 3-Cl,5-$OCH_3$ | 3.10 | | |
| 3-$OCH_3$.5-$NO_2$ | 2.11 | | | 3,5-$(OCH_3)_2$ | 3.82 | | |
| 3,5-$Br_2$ | 2.34 | | | | | | |

**NAPHTHALAMINES** (reference 88)

**substituted naphthalamines**

| **2-naphthalamine** | **X** | | | **2-naphthalamine** | **X** | | |
|---|---|---|---|---|---|---|---|
| 1-$NH_2$,3-X | $NO_2$ | 2.07 | | 2-$NH_2$,4-X | $NO_2$ | 2.43 | |
| | CN | 2.26 | | | CN | 2.66 | |
| | Cl | 2.66 | | | Cl | 3.38 | |
| | Br | 2.67 | | | Br | 3.40 | |
| | I | | 2.82 | | I | 3.41 | |
| | $COOCH_3$ | 3.12 | | | $COOCH_3$ | 3.38 | |
| | $OCH_3$ | | 3.26 | | $OCH_3$ | | 4.05 |
| | OH | 3.30 | | 1-$NH_2$,6-X | $NO_2$ | 2.89 | |
| | $CH_3$ | 3.96 | | | Cl | 3.48 | |
| | Cl | 2.71 | | | $OCH_3$ | 3.90 | |
| 2-$NH_2$,5-X | $NO_2$ | 3.01 | | | OH | 3.97 | |
| | OH | 4.07 | | 2-$NH_2$,7-X | $NO_2$ | 3.10 | |
| 1-$NH_2$,5-X | $NO_2$ | 2.73 | | | Cl | 3.71 | |
| | OH | 3.96 | | | $OCH_3$ | 4.19 | |
| | Cl | 3.34 | | | OH | 4.25 | |
| | $NH_2$ | 4.21 | | | $NH_2$ | 4.66 | |
| 1-$NH_2$,7-X | $NO_2$ | 2.55 | | 2-$NH_2$,6-X | $NO_2$ | 2.62 | |
| | Cl | 3.48 | | | $OCH_3$ | 4.64 | |
| | $OCH_3$ | | 4.07 | 2-$NH_2$,8-X | $NO_2$ | | 2.73 |
| | OH | 4.20 | | 1-$NH_2$,4-X | $NO_2$ | 0.54 | |
| 1-$NH_2$,2-X | $NO_2$ | -1.74 | | | Br | 3.21 | |
| 1-X,2-$NH_2$ | $NO_2$ | -0.85 | | 2-$NH_2$,3-X | $NO_2$ | 1.48 | |
| 1-$NH_2$,8-X | $NO_2$ | 2.79, | | | | | |

**Anilines** (in 50% ethanol)

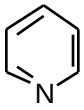
| **Unhindered** | **pK** | **ref.** |
|---|---|---|
| Aniline | 4.19 | 40 |
| p-Aminodiphenyl | 3.81 | 40 |
| 2-Naphthylamine | 3.77 | 40 |
| 3-Phenanthrylamine | 3.59 | 40 |
| m-Aminodiphenyl | 3.82 | 40 |
| 2-Aminofluorene | 4.21 | 40 |
| 2-Phenanthrylamine | 3.60 | 40 |
| 2-Anthrylamine | 3.40 | 40 |
| **Hindered** | | |
| o-Aminodiphenyl | 3.03 | 40 |
| **peri** | | |
| 1-Naphthylamine | 3.40 | 40 |
| 9-Phenanthrylamine | 3.19 | 40 |
| 3-Aminopyrene | 2.91 | 40 |
| 1-Phenanthrylamine | 3.23 | 40 |
| 1-Anthrylamine | 3.22 | 40 |
| **meso** | | |
| 9-Anthrylamine | 2.7 | 40 |
| **o-Aminophenols** | | |
| 3-Hydroxyanthranilic acid | 10.09, 5.20 | 51 |
| 2-Aminophenol hydrochloride | 9.99, 4.86 | 51 |
| **Indicators** | | |
| p-Aminoazobenzene | 2.82, 2.76 | 60 |
| 4-Chloro-2-nitroaniline | -1.02, -1.03 | 60 |
| 4,6-Dichloro-2-nitroaniline | -3.61, -3.32 | 60 |
| 6-Bromo-2,4-dinitroaniline | -6.64, -6.71 | |
| 2-Amino-4,5-dimethylphenol hydrochloride | 5.28 | 10.40, 51 |
| N,N-Dimethyl-2,4-dinitroaniline | -1.00, -- | 60 |
| p-Nitrodiphenylamine | -2.4 to -2.9, -2.50 | 60 |
| 4-Methyl-2, dinitroaniline | -3.96, -4.44 | 60 |

## Heterocyclics

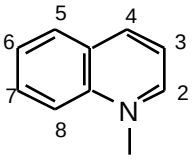
### Nucleosides, etc.

| | | |
|---|---|---|
| Adenine | 4.15, 9.80 | 6 |
| 2'-AMP | 3.81, 6.17 | 6 |
| 3'-AMP | 3.74, 5.92 | 6 |
| ADP | 3.95, 6.3 | 36 |
| ATP | 4.00 (4.1), 6.5 | 36 |
| Barbital | 7.85, 12.7 | 37 |
| Cytosine | 4.45, 12.2 | 6 |
| Cytosine (deoxy) | 4.25 | 6 |
| 3' CMP | 4.16-4.31, 6.04 | 6 |
| CDP | 4.44 | 6 |
| CDP, (deoxy) | 4.8, 6.6 | 6 |
| Guanine | 3.3, 9.2, 12.3 | 6 |
| Guanosine | 2.2, 9.5 | 6 |
| " | 1.6, 9.16, 12.5 | 35 |
| 5'-GMP | 2.4, 9.4, 6.1 | 6 |
| GDP | 2.9, 9.6, 6.3 | 6 |
| Hypoxanthine | 1.98, 8.94, 12.10 | 6 |
| 5'-IMP | 8.9, 1.54, 6.04 | 6 |
| 5-Methylcytosine | 4.6, 12.4 | 6 |
| 5-Methylcytosine deoxyriboside 5'-phosphate | 4.4 | 6 |
| 3-Methyluracil | 9.75 | 37 |
| 3-Methylxanthine | 8.5 (8.1), 11.3 | 38 |
| Adenosine | 3.63 | 6 |
| " | 3.3, 12.5 | 35 |
| 5'-AMP | 3.3, 6.1 | 36 |
| | 3.74, 6.2-6.4 | 6 |
| Barbituric acid | 3.9, 12.5 | 37 |
| Cytidine | 4.11 | 6 |
| " | 4.22, 12.5 | 35 |
| 2'-CMP | 4.3-4.4, 6.19* | 6 |
| 5'-CMP | 4.5, 6.3 | 6 |
| CTP | 4.6, 6.4 | 6 |
| 2,6-Diaminopurine | 5.09, 10.77 | 6 |
| Isoguanine | 4.51, 8.99 | 6 |
| Guanosine (deoxy) | 1.6-2.2, 9.16-9.5 | 6 |
| GMP (2' + 3') | 2.3, 9.36, 0.7, 5.9 | 6 |
| 5'-GMP (deoxy) | 2.9, 9.7, 6.4 | 6 |
| GTP | 3.3, 9.3, 6.5 | 6 |
| Inosine | 1.2, 8.9 | 6 |
| " | 8.75, 12.5 | 6 |
| 5-Methylcytosine deoxyriboside | 4.5, 13.0 | 6 |
| 1-Methyluracil | 9.95 | 37 |
| 1-Methylxanthine | 7.7, 12.05 | 38 |
| 7-Methylxanthine | 8.5 (8.3) | 38 |
| 9-Methylxanthine | 6.3 | 38 |
| Purine | 2.52, 8.90 | 37 |
| Thymidine | 9.8 | 6 |
| 5'-TMP | 10.0, 1.6, 6.5 | 6 |
| Uracil deoxyriboside | 9.3 | 6 |
| 5'-UMP | 9.5, 6.4 | 6 |
| UTP | 9.5, 6.6 | 6 |
| Uridine | 9.25 | 6 |
| " | 9.17, 12.5 | 35 |
| Xanthosine | 0, 5.5, 13.0 | 6 |
| Orotic acid | 2.8, 9.45, 13 | 6 |
| Pyrimidine | 1.30 | 37 |
| Thymine | 0, 9.9, 713.0 | 6 |
| Uracil | .5, 9.5, 13.0 | 6 |
| UMP (2' + 3') | 9.43, 1.02, 5.88 | 6 |
| UDP | 9.4, 6.5 | 6 |
| Uric acid | 5.4, 10.3 | 6 |
| Xanthine | 0.8, 7.44, 11.12 | 6 |
| " | 7.2 | 38 |

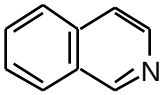
Heterocyclic Bases (Ref. 2)



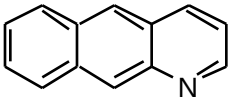
Pyridine 5.14*
pK (20°)



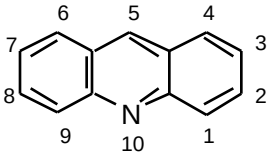
Quinoline 4.85*



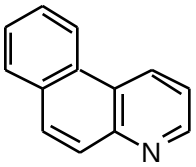
Isoquinoline 5.14*



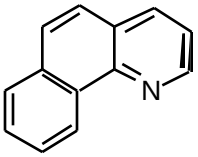
Benzoquinoline 5.05*



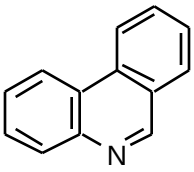
Acridine 5.60



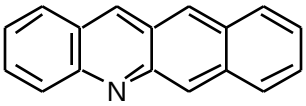
5,6-Benzoquinoline
5.15*



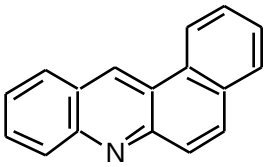
7,8-Benzoquinoline
4.25*



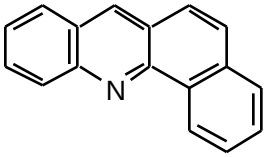
Phenanthridine 3.30[a]



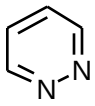
2,3-Benzacridine 4.52[a]



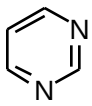
3,4-Benzacridine 4.70*



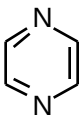
1,2-Benzacridine 3.45[a]



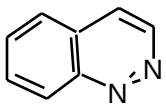
Pyridazine 2.10*



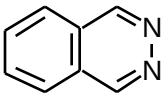
Pyrimidine 1.10*



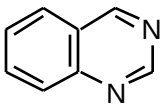
Pyrazine 0.37*



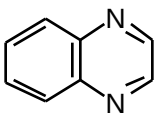
Cinnoline 2.64*



Phthalazine 3.39*



Quinazoline 3.31*



Quinoxaline 0.6*

[a] 50% EtOH

| **Heterocyclics** | | | 3-Hydroxy | 8.81, 5.52 | 39 |
|---|---|---|---|---|---|
| Aureomycin | 3.30, 7.44, 9.27 | 77 | 5-Hydroxy (acridone) | --f, -0.32 | 39 |
| Iridine | --, 5.62 | 39 | 5-Methoxy | --, 7 | 39 |

| **Acridine** | **1--** | **2--** | **3--** | **4--** | **5--** | **9--** | Ref. 2 |
|---|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| H-- | 5.60* | 4.11[a] | | | | |
| $H_2N$-- | 4.40* | 8.04* | 5.88* | 6.04* | 9.99* | |
| | 3.59[a] | 7.61[a] | 5.03[a] | 5.50[a] | 9.45[a] | |
| HO-- | 4.18[a] | 4.86[a] | 5.52[39] | 4.45[a] | -.32[39] | |
| | 10.7[a] | 9.9[a] | 8.81[39] | 9.4* | >12 | |
| $CH_3$-- | 3.95[a] | | 4.60[a] | | 4.70[a] | |
| $H_2K$-(1-$CH_3$--)-- | | | | 4.79[a] | 9.73[s] | 3.22[a] |
| 1,9-$(CH_3)_2$-- | 2.88[a] | | | | | |

[a] 50% ethanol; ref. 39

| | | |
|---|---|---|
| 8-amino-1,2-benzacridine | 6.72 | 40 |
| 2-amino-4-methyl-5,6-benzoquinoline | 7.14 | 40 |
| 3-amino-6,7-benzoquinoline | 4.78 | 40 |
| 8-amino-3,4-benzacridine | 7.42 | 40 |
| 1'-amino-5,6-benzoquinoline | 5.03 | 40 |
| 4'-amino-5,6-benzoquinoline | 5.20 | 40 |
| 2-amino-4-methyl-7,8,benzoquinoline | 6.74 | 40 |
| 6,7-benzoquinoline | 5.05, 3.84[a] | 19 |
| 5,6-benzoquinoline | 5.15, 3.90[a] | 19 |
| 4-amino- | 7.99[a] | 19 |
| 2-methyl- | 4.44[a] | 19 |
| 4-amino-2-methyl- | 8.45[a] | 19 |
| 2-amino-4-methyl- | 7.14, 6.51[a] | 19 |
| 4'-amino- | 5.20, 4.10[a] | 19 |
| 3'-amino- | 4.02[a] | 19 |
| 1'-amino- | 5.03 | 19 |
| 2',4'-diamino- | 4.91[a] | 19 |
| Benziminazole | 5.53 | 19 |
| 2-amino- | 7.54 | 19 |
| Benztriazole | 1.6 | 19 |
| Benzthiazole | 1.2, 0.1[a] | 19 |
| 2-amino- | 4.51 | 19 |
| benzoxazole | (decomp.) | 19 |
| 2-amino- | 3.73 | 19 |
| 2,3-benzacridine | 4.52[a] | 19 |
| 5-amino- | 9.72[a] | 19 |
| 5-acetamido- | 4.56[a] | 19 |
| 7-amino- | 5.38[a] | 19 |
| 5-amino-6:7:8:9-tetrahydro- | 9.66[a] | 19 |
| Caffeine | 0.61 | 4 |
| cinchonine | 7.2 | 4 |
| Cinnoline | 2.70 | 19 |
| 4-amino- | 6.84 | 19 |
| Cocaine | 7.6 | 4 |
| Cinnoline 4-hydroxy | 9.27, 0.35 | 39 |
| 6-hydroxy | 7.52, 3.65 | 39 |
| -hydroxy | 8.20, 2.74 | 39 |

| | | |
|---|---|---|
| α,α'-dipyridyl | 4.43 | 6 |
| 4-amino- | 8.75[a] | 19 |
| 4-amino-2-methyl- | 9.45[a] | 19 |
| 4-amino-2-methyl-8-chloro- | 5.95[a] | 19 |
| 8-chloro- | 2.5[a] | 19 |
| 3,4-diamino- | 8.15[a] | 19 |
| 3-amino- | 4.78, 3.73[a] | 19 |
| 7,8-benzquinoline | 4.25, 3.15[a] | 19 |
| 4-amino- | 7.68[a] | 19 |
| 4-amino-2-methyl- | 7.96[a] | 19 |
| 2-amino-4-methyl- | 6.74, 6.02[a] | 19 |
| 6-amino-2-methyl- | 5.23[a] | 19 |
| 1'-amino-2-methyl- | 4.75[a] | 19 |
| 3,4-benzacridine | 4.70, 4.16[a] | 19 |
| 5-amino | 8.41[a] | 19 |
| 7-amino- | 5.03[a] | 19 |
| 8-amino- | 7.42 (6.51)[a] | 19 |
| 8-acetamido- | 4.48[a] | 19 |
| 8-dimethylamino- | 7.31, 6.99 | 19 |
| 1,2-benzacridine | 3.45[a] | 19 |
| 5-amino- | 8.13[a] | 19 |
| 7-amino | 4.05[a] | 19 |
| 8-amino- | 6.72, 5.97[a] | 19 |
| 4',5-diamino- | 8.44[a] | 19 |
| Cinnoline | --, 0.21 | 39 |
| 3-hydroxy | 8.64, 0.21 | 39 |
| 5-hydroxy | 7.40, 1.92 | 39 |
| 7-hydroxy | 7.56, 3.31 | 39 |
| 4-methoxy | --, 3.21 | 39 |

**Heterocyclics**

| | | |
|---|---|---|
| o,o'-dipyridyl | 4.43 | 6 |
| **hydantoin** | 9.16 | 42 |
| 5-isopropyl-2-thio- | 8.70 | 42 |
| 5,5-pentamethylene2-thio | 8.79 | 42 |
| 3,5,5-trimethyl-2-thio | 10.80 | 42 |
| 3-methyl-5,5-pentamethylene-2-thio- | 11.23 | 42 |

**Imidazoles**

| | | |
|---|---|---|
| 2-Methylimidazole | 7.75 | 43 |
| N-Acetylhistidine | 7.05 | 43 |
| 2-Methyl-4-hydroxy-aminobenz- | 6.65 | 43 |
| 4-Hydroxymethyl- | 6.45 | 43 |
| 2-Methylbenz- | 6.1 | 43 |
| Histamine | 6.0 | 43 |
| 4-Hydroxy-6-aminobenz- | 5.9 | 43 |
| 4-Hydroxybenz- | 5.3 (OH 9.5) | 43 |
| 4-Methoxybenz- | 5.1 | 43 |
| 4-Bromo- | 3.7 | 43 |
| 6-Nitrobenz- | 3.05, 10.6 | 43 |
| 4-Nitro- | 1.5, 9.1 | 43 |
| **isoQuinolines** | | |
| 1-Hydroxy- | -1.2 | 44 |
| 5-Hydroxy | 5.40, 8.45 | 44 |
| 3-Amino- | 5.05 | 40 |
| 5-Amino- | 5.59 | 40 |
| Amino- | 6.20 | 40 |
| 6-Hydroxy- | 5.85, 9.15 | 44 |
| 8-Hydroxy- | 5.66, 8.40 | 44 |
| 2-Methylisoquinolone | -1.8 | 44 |
| Isoquinoline | 5.46, 5.14 | 44, 19 |
| Phenazine | --, 1.23 | 39 |
| 2-Hydroxy- | 7.5, 2.6 | 39 |
| 10-Methyl-2-phenazone | --, 3.0 | |
| 6-Aminophenanthridine | 6.88 | 40 |
| 9-Aminophenanthridine | 7.31 | 40 |
| o-Phenanthroline | 4.27[a], 5.2 | 19 |
| p-Phenanthroline | 3.12[a] | 19 |
| 1,10-Diamino-3,8-Dimethyl- | 8.78[a], 6.31[a] | |
| Phenanthridine | --, 4.65 | 44 |
| 6-Hydroxy- | 8.43, 5.35 | 44 |
| 9-Hydroxy (phenanthridone) | <-1.5 | 44 |
| 9-Amino- | 7.31, 6.75[a] | 19 |
| 2,7,9-Triamino- | 8.06[a] | 19 |
| Phthalazine | 3.47 | 19 |
| 1-Amino- | 6.60 | 19 |
| 1-Hydroxy- | 11.00, -2 | 39 |
| Picolimic acid | 5.52 | 4 |
| 5,5-dimethyl-2-thio- | 8.71 | 42 |
| 5,5-Diphenyl-2-thio- | 7.69 | 42 |
| 1-Methyl-5,5-pentamethyl-ene-2-thio- | 9.25 | 42 |
| 4-Methyl- | 7.45 | 43 |
| Imidazole | 6.95 | 43 |
| 4-(2',4'-Dihydroxyphenyl)- | 6.45 | 43 |
| Carbobenzoxy-L-histidyl-L-tyrosine ethyl ester | 6.25 | 43 |
| 6-Aminobenz- | 6.0 ($NH_2$ 3.0) | |
| Benzimidazole | 5.4 | 43 |
| Histidine methylester | 5.2 ($NH_2$ 7.1) | 43 |
| 2-Methyl-4-hydroxy-6-nitro-benzimidazole | 3.9 | 43 |
| 4-Hydroxy-6-Nitrobenz- | 3.05 | 43 |
| [b]2-Hydroxymethylnaphth(1,2)- | 4.44, 12.23 | 86 |
| [b]2-Hydroxymethylnaphth(2,3)- | 4.50, 12.23 | 86 |
| 4-Hydroxy- | 4.80, 8.68 | 44 |
| 1-Amino- | 7.62 | 40 |
| 4-Amino- | 6.28 | 40 |
| 6-Amino- | 7.17 | 40 |
| 8-Amino- | 6.06 | 40 |
| 7-Hydroxy- | 5.70 | 40 |
| 1-Methoxy- | 3.05 | 44 |
| 4-$NO_2$ | 1.35 | 88 |
| 4-Br | 3.31 | 88 |
| 1-Hydroxy- | --, 1.44 | 39 |
| 5-Methyl-1-phenazone | --, 4.9 | 39 |
| m-Phenanthroline | 3.11[a] | 19 |
| 1-Amino- | ca. 7.3, 7.29[a] | 19 |
| 2,2'-Dipyridyl | 4.23 | 19 |
| 2-Hydroxy- | 8.79, 4.82 | 44 |
| 7-Hydroxy- | 4.38, 8.68 | 44 |
| 9-Methoxy- | --, 2.38 | 44 |
| 2-Amino-9-methyl- | 5.66[a] | 19 |
| 2,7-Diamino-9-methyl- | 6.26[a] | 19 |
| 6-Amino- | 6.88 | 40 |
| Phenazine | 1.23 | 19 |
| 1-Amino- | 2.6[a] | 19 |
| 2-Amino- | 4.75, 3.46[a] | 19 |
| 1,3-Diamino- | 5.64[a] | 19 |
| 2,3-Diamino- | 4.74 | 19 |
| 2,7-Diamino- | 4.63, 3.9[a] | 19 |
| Pteroylglutamic acid | 8.26 | 77 |
| **Pyridines** | | |
| 2-Amino- | 6.86 | 41 |
| 4-Amino- | 9.17 | 41 |
| 2-Methyl- | 5.94[b] | 45 |
| 2-Vinyl- | 4.98 | 45 |
| 2-Chloro- | 0.49 | 45 |
| 2,4,6-Trihydroxy- | 4,6, 9.0, 13 | 39 |
| 1-Methyl-4-pyridone | 3.33 | |
| 2-(N-Methylacetamido)- | 2.01 | 46 |
| 2-Benzamido- | 3.33 | |
| 2-(N-Methylbenzamido)- | 1.44 | |
| 3-(N-Methylacetamod)- | 3.52 | 46 |
| 3-(N-Methylbenzamido)- | 3.66 | 46 |
| 4-(N-Methylacetamido)- | 4.62 | 46 |

| | | |
|---|---|---|
| 4-(N-Methylbenzamido)- | 4.68 | 46 |
| 4-Benzamido- | 5.32 | 46 |
| 3-$NO_2$ | 0.81 | 88 |
| 3-$COO^-$ | 4.77 | 47 |
| 2,3-$Me_2$ | 6.60 | 48 |
| 2,5-$Me_2$ | 6.47 | 48 |
| 3,4-$Me_2$ | 6.52 | 48 |
| 2,4,6-$Me_3$ | 7.48 | 48 |
| 4-OEt | 6.67 | 48 |
| 3-Cl | 2.84 | 48 |
| 3-$CO_2$Et | 3.35 | 48 |
| 3-COOH | 3.13 | 88 |
| 2-Amyl- | 6.00[b] | 45 |
| 2-Hexyl- | 5.95[b] | 45 |
| 2-Benzyl- | 5.13 | 45 |
| 2-Bromo- | 0.71 | 45 |
| 2,4-Dihydroxy | 6.50, 13, 1.37 | 39 |
| 1-Methyl-2-pyridone | 0.32 | 39 |
| 2-Acetamido- | 4.09 | 46 |
| 1-Methylpyrid-2-one acetylimine | 7.12 | 46 |
| 3-Acetamido- | 4.46 | 46 |
| 3-Benzamido- | 3.80 | 46 |
| 1-Methylpyrid-4-one acetylimine | 11.03 | 46 |
| 1-Methylpyrid-4-one benzylimine | 9.89 | 46 |
| 4-$COO^-$ | 4.90 | 47 |
| 2,4-$Me_2$ | 6.72 | 48 |
| 2,6-$Me_2$ | 6.77 | 48 |
| 3,5-$Me_2$ | 6.14 | 48 |
| 2-Me,5-Et | 6.51 | 48 |
| 3-F | 3.10 | 48 |
| 3-Br | 2.84 | 48 |
| 4-$CO_2$Et | 3.45 | 48 |

*Pyridine N-oxides (see oxygen acids)*

**Substituted Pyridines**

| **Pyridine** | **2-** | **3-** | **4-** |
|---|---|---|---|
| H- | 5.17[b] | | |
| Cl- | 0.72[b] | 2.84[b] | |
| I- | 1.82[b] | 3.25[b] | |
| $CH_3CH_2$- | 5.97[b] | 5.70[b] | 6.02[b] |
| $(CH_3)_3C$- | 5.76[b] | 5.82[b] | 5.99[b] |
| HO- | 0.75 | 4.86 | 3.27 |
| | 11.62 | 8.72 | 11.09 |
| $SO_3$-[47] | | 2.9 | |
| $CH_3O$- | 3.28 | 4.88 | 6.62 |
| F- | -0.44[b] | 2.97[b] | |
| Br- | 0.90[b] | 2.84[b] | |
| $CH_3$- | 5.97[b] | 5.68[b] | 6.02[b] |
| $(CH_3)_2CH$- | 5.83[b] | 5.72[b] | 6.02[b] |
| $CH_3CO$ | | 3.18[b] | |
| $H_2N$- | 6.68[b] | 5.80[b] | 8.96[b] |
| $CONH_2$[47] | | 3.40 | 3.61 |
| NC-[47] | | 1.45 | |

**Ortho-Substituted Pyridines** (in 50% ethanol)

| **Substituent** | **pK** | **ref.** |
|---|---|---|
| H- | 4.38 | 2 |
| 2-$C_2H_5$- | 4.93 | 2 |
| 2-($CH_3$) | 4.68 | 2 |
| 2,6-[$(CH_3)_2CH]_2$ | 3.58 | 2 |
| 2-$(CH_3)_3C$- | 4.68 | 2 |
| 2-$C_2H_5$-6-$(CH_3)_3C$- | 4.36 | 2 |
| 2,6-$[(CH_3)_3C]_2$– | 3.58 | 2 |
| 2-$CH_3$- | 5.05 | 2 |
| 2-$(CH_3)_2CH$- | 4.82 | 2 |
| 2,6-$(CH_3)_2$ | 5.77 | 2 |
| 2,6-$[(CH_3)_3C]_2$ | 3.58 | 2 |
| 2-$CH_3$-6-$(CH_3)_3C$ | 5.52 | 2 |
| 2-$(CH_3)_2CH$-6-$(CH_3)_3C$- | 5.13 | 2 |

| | | **$pK_{NH}$** | **35°** | **$pK_{OH}$** | |
|---|---|---|---|---|---|
| Benzimidazole | 6.00 | 5.58 | 5.36 | | |
| 2-Methyl | 6.96 | 6.29 | 6.18 | --- | |
| 2-Ethyl | 6.90 | 6.27 | 6.14 | -- | |
| 2-Hydroxymethyl | --- | 5.40 | --- | 11.55 | ref. 86 |
| 1-Methyl-2-hydroxymethyl | --- | 5.55 | --- | 11.45 | |

**Other** (ref. 95)

| | |
|---|---|
| Thiazolidine | 6.31 |
| Methyl thiazolidine-4-carboxylate | 4.00 |
| Thiazolidine-4-COOH | 1.51, 6.21 |

(ref. 96)

| | |
|---|---|
| 2-Methyl-$\Delta^2$-oxazoline | 5.5 |
| 4-Carbamoyl-2-phenyl-$\Delta^2$-oxazoline | 2.9 |
| 2-Phenyl-$\Delta^2$-oxazoline | 4.4 |

**Heterocyclics**

| **Pyrazines** | **pK** | **ref**. |
|---|---|---|
| Pyrazine | 1.1, 0.6 | 49, 39 |
| 2,5-Dimethyl- | 2.1 | 49 |
| 2,3,5,6-Tetramethyl- | 2.8 | 49 |
| 2-Methoxy- | --, 0.75 | 39 |
| 2-Methyl- | 1.5 | 49 |
| 2,6-Dimethyl- | 2.5 | 49 |
| 2-Hydroxy- | 8.23, 0.1 | 39 |
| 1-Methyl-2-pyrazine | -0.04 | 39 |
| 2-Amino- | 3.14 | 19 |
| Pyrimidine | 1.30 | 19 |
| 2-Amino- | 3.54 | 19 |
| 5-Amino- | 2.83 | 19 |
| 2-Amino-4,6-dimethyl- | 4.85 | 19 |
| 2,4,6-Triamino- | 6.84 | 19 |
| 2-Hydroxy- | 9.17, 2.24 | 39 |
| Pyridazine | 2.33 | 19 |
| 3-Hydroxy- | 10.46, -1.8 | 39 |
| 3,6-Dihydroxy- | 5,67, -2.2, 13 | 39 |
| 4-Methoxy- | 3.70 | 39 |
| 3-Amino- | 5.19 | 19 |
| 4-Hydroxy- | 8.68, 1.07 | 39 |
| 3-Methoxy- | 2.52 | 39 |
| 3,6-Dimethoxy- | 1.61 | 39 |

*For complex chelating agents, see also ref. 77*
*[b] thermodynamic at 25°.*

| | | |
|---|---|---|
| 2,4-Dihydroxy-(Uracil) | 9.38, 12 | 39 |
| 4,6-Dihydroxy- | 5.4 | 39 |
| 2,4,6-Trihydroxy-(Barbituric acid) | 3.9, 12.5 | 39 |
| 2-Methoxy- | <1 | 39 |
| 4-Methoxy- | 2.5 | 39 |
| 1-Methyl-2-pyrimidone | 2.50 | 39 |
| 3-Methyl-4-pyrimidone | 1.84 | 39 |
| 4-Amino- | 5.71 | 19 |
| 2-Amino-4-methyl- | 4.15 | 19 |
| 2,4-Diamino- | 7.26 | 19 |
| 4-Methyl- | 1.98 | 19 |
| 4-Hydroxy- | 8.59, 1.85 | 39 |
| 4,5-Dihydroxy- | 7.48, 1.99, 11.61 | 39 |
| 2,4,5-Trihydroxy-(isoBarbituric acid) | 8.11, 11.48 | 39 |
| 4-Hydroxy-5-methoxy- | 8.60 | 1.75 39 |
| 1-Methyl-4-pyrimidone | 1.8 | 39 |

**Miscellaneous**

| | | |
|---|---|---|
| 4-Hydroxy-2-methylpyridazinium chloride | 1.74 | 44 |
| 8-Hydroxy-6-methyl-1,6-naphthyridinium chloride | 4.34 | 44 |
| 2-Hydroxyphenazine | 2.6 | 44 |
| 4-Hydroxypteridine | -0.17 | 44 |
| 3-Methyl-4-pteridone | -0.47 | 44 |
| 5-Hydroxypyrimidine | 1.87, 6.78 | 44 |
| 8-Hydroxy-1,6-Naphthyridine | 4.08 | 44 |
| 1-Hydroxyphenazine | 1.44 | 44 |

| | | |
|---|---|---|
| 5-Methyl-1-phenazone | 4.9 | 44 |
| 10-Methyl-2-phenazone | 3.0 | 44 |
| 1-Methyl-4-pteridone | 1.25 | 44 |

| **Quinoline** | **2--** | **3** | **4** | **5** | **6** | **7** | **8** | **Ref.** |
|---|---|---|---|---|---|---|---|---|
| H- | 4.85* | 4.80 | 4.69* | | | | | 2 |
| $H_2N$- | 7.25* | 4.86* | 9.08* | 5.37* | 5.54* | 6.56* | 3.90* | 2 |
| HO- | -.36 | 4.30 | 2.27 | 5.20 | 5.17 | 5.48 | 5.13 | 44 |
| | 11.74 | 8.06 | 11.25 | 8.54 | 8.88 | 8.85 | 9.89 | 44 |
| $CH_3$ | 5.42 | 5.14 | 5.20 | 4.62 | 4.92 | 5.08 | 4.60 | 2 |
| | 5.8 | | 5.6 | | 5.2 | | 5.0 | 2 |
| F- | | 2.36* | | 3.68* | 4.00* | 4.04* | 3.08* | 2 |
| Cl- | | | | | 3.73* | | | 2 |
| $HO_2C$ | 4.96* | 4.62* | 4.53* | 4.81* | 4.98* | 4.97* | 7.20* | 2 |
| $NO_2$ | | $1.03^{88}$ | | | | | | |

| **Quinoline** | | |
|---|---|---|
| 2,4-Dihydroxy- | 5.86, 0.76 | 39 |
| 4-Methoxy- | 6.65 | 59 |
| 1-Methyl-4-quinolone | 2.46 | 39 |
| 2,4-Diamino- | 9.45 | 19 |
| **Quinazoline** | 3.51, 3.2[a] | 19 |
| 2-Amino- | 4.43 | 19 |
| 6-Amino- | 3.2[a] | 19 |
| 2-Hydroxy- | 10.69, 1.30 | 39 |
| 6-Hydroxy- | 8.19, 3.12 | 39 |
| 3-Methiodide | 7.26 | 39 |
| 2-Methoxy- | 1.31 | 39 |
| 2-Methoxy- | 3.17 | 39 |
| 1-Methyl-2-quinolone | -0.71 | 39 |
| 4-Amino- | 9.44, 9.17 | 19, 41 |
| 8-Quinolinol | 5.13, 9.89 | 6 |
| 3-Cl | --, 2.46 | 88, 44 |
| 3-Br | 2.61 | 88 |
| 4-Amino- | 5.73 | 19 |
| 8-Amono- | 2.4[a] | 19 |
| 4-Hydroxy- | 9.81, 2.12 | 39 |
| 8-Hydroxy- | 8.65, 3.41 | 39 |
| 2,4-Dihydroxy- | 9.78, 2.5 | 39 |
| 4-Methoxy- | 3.13 | 39 |

*Thermodynamic

| **Heterocyclics** | | |
|---|---|---|
| **Quinoxaline** | 0.8, 0.56 | 19, 39 |
| 2-Amino- | 3.96 | 19 |
| 6-Amino- | 2.95 | 19 |
| 2-Hydroxy- | 9.08, -1.37 | 39 |
| 1-Methiodide | 5.74 | 39 |
| 2,3-Dihydroxy- | 9.52 | 39 |
| 5-Hydroxy-1-methylquioxalinium chloride | 5.74 | 44 |
| Riboflavin | 9.93 | 77 |
| Sulphadiazine | 6.48 | 6 |
| Sulphapyridine | 8.43 | 6 |
| 2-Aminothiazole | 5.39 | 41 |
| 1,3,5-Triazine | -- | 39 |
| 2,4-Dihydroxy- | 6.5 | 39 |
| 1,4,6-Triazanaphthalene | 2.5 | 39 |
| 4-Hydroxy- | 11.05, 0.78 | 39 |
| 5-Amino- | 2.62 | 19 |
| 2,3-Diamino- | 4.70 | 19 |
| 5-Hydroxy- | 8.65, 0.9 | 39 |
| 6-Hydroxy- | 7.92, 1.40 | 39 |
| 1,5-Naphthyridine | 2.91 | 39 |
| 4-Hydroxy | 10.01, 2.85 | 39 |
| Sulphaquanidine | 11.25 | 6 |
| Sulphathiazole | 7.12 | 6 |
| Terramycin | 3.10, 7.26, 9.11 | 77 |
| Tetramethylenediamine | 10.7 | 4 |
| 1,4,5-Triazanaphthalene | 1.20 | 39 |
| 8-Hydroxy- | 8.76, 0.60 | 39 |

## SPECIAL NITROGEN COMPOUNDS

| **Hydroxylamines** | | |
|---|---|---|
| Hydroxylamine | 5.97* | 12 |
| N-Methyl- | 5.96* | 12 |
| O-Methyl- | 4.60* | 12 |
| Trimethyl- | 3.65* | 12 |
| N-Dimethyl- | 5.20* | 12 |
| N,O-Dimethyl- | 4.75* | 12 |

**Hydrazines (30°)**

| | | |
|---|---|---|
| Hydrazine | 8.07 | 13 |
| Methyl- | 7.87 | 13 |
| N,N'-Dimethyl- | 7.52 | 13 |
| Tetramethyl- | 6.30 | 13 |
| N,N-Diethyl- | 7.71 | 13 |
| Phenyl- | 5.21 (15°) | 14 |
| Glycylhydrazide | 2.38, 7.69 | 15 |
| N,N-Dimethyl- | 7.21 | 13 |
| Trimethyl- | 6.56 | 13 |
| Ethyl- | 7.99 | 13 |
| N,N'-Diethyl- | 7.78 | 13 |
| Acet- | 3.24 | 15 |
| Isonicotinhydrazide | 1.85, 3.54, 10.77 | 77 |

**Hydrazones** Hydrazone of:

| | | |
|---|---|---|
| Benzophenone | 3.85 | 16 |
| p,p'-Dimethoxy- | 4.38 | 16 |
| p-Chloro- | 4.38 | 16 |
| p-Methoxyacetophenone | 4.94 | 16 |
| p,p'-Dichloro- | 3.13 | 16 |
| Phenyl-2-thienyl ketone | 3.80 | 16 |

**Semicarbazones** of:

| | | |
|---|---|---|
| Semicarbazide | 3.66 | |
| Furfural | 1.44 | 14 |
| Benzaldehyde | 0.96 | 14 |
| Acetone | 1.33 | 14 |
| Acetaldehyde | 1.10 | 14 |
| Pyruvic acid | 0.59 | 14 |

**Amidoximes**

| | | |
|---|---|---|
| Ox- | 3.02 | 17 |
| Benz- | 4.99 | 17 |
| α-Phenylacet- | 5.24 | 17 |
| Succin- | 3.11, 5.97 | 17 |
| o-Tolu- | 4.03 | 17 |
| p-Tolu- | 5.14 | 17 |
| Malon- | ~4.77 | 17 |

**Other**

| | | |
|---|---|---|
| Diphenylthiocarbazone | 4.5 | 6 |
| Phthalimide | 8.30 | 18 |
| Nitrourethane | 3.28 | 18 |
| Acetylguanidine | 8.33 | 19 |
| Acetamidine | 12.52 | 19 |
| O-Methylisourea | 9.80 | 20 |
| Dimedone | 5.23 | 18 |
| Nitrourea | 4.57 | 18 |
| Guanidine | 13.71 | 19 |
| Phenylguanidine | 10.88 | 19 |
| Benzamidine | 11.6 | 19 |
| N-Phenyl-O-methylisourea | 7.3 | 20 |

**Nitrogen compounds, miscellaneous**

| | | |
|---|---|---|
| Diguanide$^{--}$ | 3.07, 13.25 | 77 |
| Dithiooxamide (rubeanic acid, $H_2NCSCSNH_2$) | 10.62 | 77 |
| Ethylenediguanide | 1.74, 2.88, 11.34, 11.76 | 77 |
| Phenyldiguanide | 2.16, 10.71 | 77 |

**Other**

| | | |
|---|---|---|
| S-Methylisothiourea | 9.83 | 20 |
| N-Phenyl-S-methylisothiourea | 7.14 | 20 |

**Cinchona Alkaloids** (in 80% aqueous methyl cellosolve)

| | | |
|---|---|---|
| Quinine | 7.73 | 2 |
| Quinidine | 7.95 | 2 |
| Ephedrine | 9.14 | 2 |
| N-Methylephedrine | 8.50 | 2 |
| Epiquinine | 8.44 | 2 |
| Epiquinidine | 8.32 | 2 |
| ψ-Ephedrine | 9.22 | 2 |
| N-Methyl-ψ-ephedrine | 8.81 | 2 |

| | | |
|---|---|---|
| Acetamide | -0.51 | 4 |
| Urea | 0.18 | 4 |
| Thiourea | -0.96 | 4 |

**Thiols**

| | | |
|---|---|---|
| N-Dimethyl-cysteamine | 7.95, 10.7 | 7 |
| N-Dipropyl-cysteamine | 8.00 10.8 | 5 |
| N-β-Mercaptoethyl-morpholine | 6.65, 9.8 | |
| 1-Diethylamino-butan- (4) | 10.1 | 5 |
| Methyl-[β-diethylamino-ethyl]-sulfide | 9.8 | 5 |
| Methyl thioglycolate | 7.8 | 23 |
| Mercaptoethylamine | 8.6, 10.75 | 23 |
| N-trimethyl cysteine | 8.6 | 23 |
| Glutathione | 2.12, 3.59, 8.75, 9.65 | 23 |
| N-Diethyl-cysteamine | 7.8, 10.75 | 5 |
| N-B-Mercaptoethyl-piperidine | 7.95, 11.05 | 5 |
| 1-Diethylamino-propan- (3) | 8.0, 10.5 | 5 |
| 1-Diethylamino-hexan- (6) | 10.1 | 5 |

| | | |
|---|---|---|
| p-Nitrobenzenethiol | 5.1 | 58 |
| Thioglycolic acid | 3.67, 10.31 | 23 |
| Mercaptoethanol | 9.5 | 23 |
| Cysteine | 1.8, 8.3, 10.8 | 23 |
| Cysteinylcysteine | 2.65, 7.27, 9.35, 10.85 | 23 |

| **X=** | **-H** | **-S⁻** | **-SH** |
|---|---|---|---|
| $X(CH_2)_2SH$ | 12.0 | 13.96 | 10.75 |
| $X(CH_2)_4SH$ | 12.4 | 13.25 | 11.50 |
| $X(CH_2)_3SH$ | 13.24 | 11.14 | |
| $X(CH_2)_5SH$ | | 13.27 | 11.82 |

| | | |
|---|---|---|
| o-Mercapto-phenylacetic acid | 4.28, 7.67 | 59 |
| Ethyl mercaptan | 10.50 | 81 |
| I-Thio-D-sorbitol | 9.35 | 91 |
| 2-mercaptoethanesulfonate | 7.53 (9.1) | 81 |
| o-aminothiophenol | 6.59 | 81 |
| Thiophenol | 8.20[a], 7.8, 6.52 | 59, 81, 82 |
| B-Mercaptopropionic acid | 10.27 | 81 |
| Methyl cysteine | 6.5 (7.5) 81 | |
| p-Cl-thiophenol | 7.50 | 81 |

**Mercaptans, RSH**

| **R** | | |
|---|---|---|
| $CH_3CCH_2$- | 7.86 | 32 |
| $C_6H_5CH_2$- | 9.43 | 82 |
| $HOCH_2CH(OH)CH_2$- | 9.51 | 82 |
| $CH_2$=$CHCH_2$- | 9.96 | 82 |
| n-$C_4H_9$- | 10.66 | 82 |
| t-$C_5H_{11}$- | 11.21 | 82 |
| $C_2H_5OCOCH_2$- | 7.95 | 82 |
| $C_2H_5OCH_2CH_2$- | 9.38 | 82 |
| $HOCH_2CH(OH)CH_2$- | 9.66 | 82 |
| n-$C_3H_7$- | a10.65 | 82 |
| t-$C_4H_9$- | 11.05 | 82 |

**CARBON ACIDS**

| | | |
|---|---|---|
| Acetone | ~20 | 24 |
| Acetylacetone | 8.95 | 24 |
| Diacetylacetone | 6 | 24 |
| Hydrocyanic acid | 9.21 | 25 |
| 1-nitropropane | 9 | 18 |
| Saccharin | 1.6 | 18 |
| Tri-methylsulfonyl-methane | strong | 24 |
| Dicyanomethane | 12 | 2 |
| Acetonitrile | c. 25 | 24 |
| Benzoylacetone (anol) | 8.23 | 24 |
| Dimethylsulfone | 14 | 24 |
| Nitroethane | 8.6 | 18 |
| 2-nitropropane | 7.74 | 18 |
| Tricyanomethane | strong | 24 |
| Trinitromethane | strong | 24 |
| Nitromethane | strong | 25 |

**Bis-(β-Diketones):$[(RCO)(R'CO)CH]_2CHR$ (**in 50% dioxane) (ref. 28)

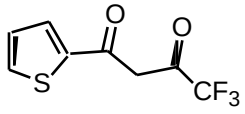
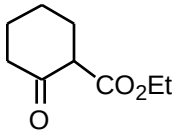
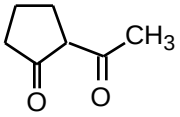
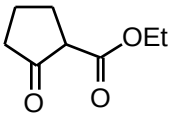
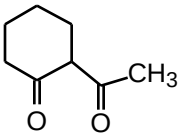
| **R** | **R'** | **R"** | **pK** | **pK** |
|---|---|---|---|---|
| $CH_3$ | $CH_3$ | $(CH_2)_5CH_3$ | 11.33 | 12.52 |
| $CH_3$ | $CH_3$ | $C_6H_5$ | 11.10 | 12.49 |
| $CH_3$ | $CH_3$ | 2-$ClC_6H_4$ | 11.04 | 12.73 |
| $CH_3$ | $CH_3$ | 2-$C_5H_4N$ | 9.80 | 12.46 |
| $CH_3$ | $CH_3$ | 2-$CH_3OC_6H_4$ | 11.47 | 12.44 |
| $CH_3$ | $CH_3$ | 3,4-$CH_2O_2C_6H_3$ | 11.39 | 12.60 |
| $CH_3$ | $CH_3$ | 3-$C_5H_4N$ | 10.29 | 12.63 |
| $CH_3$ | $CH_3$ | 4-$CH_3OC_6H_4$ | 11.62 | 12.61 |
| $CH_3$ | $CH_3$ | 4-$(CH_3)_2NC_6H_4$ | 11.50 | 12.45 |
| $CH_3$ | $CH_3OCH_2$ | $C_6H_5$ | 11.54 | 12.27 |
| $CH_3$ | $CH_3OCH_2$ | 2-$C_5H_4N$ | 10.95 | 12.49 |
| $CH_3$ | $CH_3OCH_2$ | 4-$(CH_3)_2NC_6H_4$ | 12.13 | 12.31 |
| $CH_3$ | $CH_3OCH_2$ | 4-$CH_3OC_6H_4$ | 11.74 | 12.49 |
| | $CH_3OCH_2COCH_2COCH_3$ | | 9.66 | |
| | $(CH_3CO)_2CH(CH_2)_3CH_3$ | | 12.07 | |

**Bis-(β-Diketones) (RCO)-(R'CO)CH-Y-CH(COR)(COR')** (in 50% dioxane) (ref. 26)

| R | R' | Y | pK | pK |
|---|---|---|---|---|
| $CH_3$ | $CH_3$ | | 9.43 | 13.54 |
| $CH_3$ | $CH_3$ | $(CH_2)_4$ | 11.99 | 12.48 |
| $CH_3$ | $CH_3$ | $(CH_2)_{10}$ | 12.01 | 12.07 |
| $CH_3$ | $CH_3$ | 1,4-$(CH_3)_2C_6H_4$ | 11.27 | 12.15 |

**Bis-(β-Diketones) $RCOCH_2CO$-Y-$COCH_2COR$** (in 75% dioxane) (ref. 26)

| **R** | **Y** | **pK** | **pK** |
|---|---|---|---|
| $C_6H_5$ | $(CH_2)_4$ | 12.47 | 13.09 |
| $C_6H_5$ | $(CH_2)_5$ | 12.72 | 13.46 |
| $C_6H_5$ | $(CH_2)_6$ | 12.60 | 13.46 |
| $C_6H_5$ | $(CH_2)_7$ | 13.1 (est.) | |
| $C_6H_5$ | $(CH_2)_3$ | 12.58 | 13.69 |
| $CH_3$ | $(CH_2)_5$ | 12.29 | 13.00 |
| $CH_3$=$CH(CH_3)_2$ | $(CH_2)_5$ | 12.95 | 13.60 |

| | | |
|---|---|---|
| $CH_3NO_2$ | 10.29 | 74 |
| $CH_3CHClNO_2$ | 7 | 74 |
| $CH_3COCH_2\ NO2$ | 5.1 | 74 |
| $CH(NO_2)_3$ | strong | 74 |
| $CH_3COCHCl_2$ | 15 | 74 |
| $CH_3COCHC_2H_5CO_2C_2H_5$ | 12.7 | 74 |
| $CH_3COCHCH_3COCH_3$ | 11 | 74 |
| $CH_3COCH_2COC_6H_5$ | 9.4 | 74 |
| $C_6H_5COCH_2COCF_3$ | 6.82 | 74 |
| $CH_3COCH_2CHO$ | 5.92 | 74 |
| $CH_3\ COCH2\ CO2CH_3$ | 10 | 74 |
| $CH_3SO_2CH_2SO_2CH_3$ | 14 | 74 |
| $CH_3SO_2CH(COCH_3)_2$ | 4.3 | 74 |
| $C_2H_5NO_2$ | 8.6 | 74 |
| $C_2H_5O_2CCH_2\ NO2$ | 5.82 | 74 |
| $CH_2(NO_2)_2$ | 3.57 | 74 |
| $CH_3COCH_2Cl$ | c. 16.5 | 74 |
| $CH_3COCH_2CO_2C_2H_5$ | 10.68 | 74 |
| $CH_3COCH_2COCH_3$ | 9 | 74 |
| $CH_3COCHBrCOCH_3$ | 7 | 74 |
| $CH_3COCH_2COCF_3$ | 4.7 | 74 |
| $C_6H_5COCH_2NC_5H_5$ | 10.51 | 74 |
| $CH(COCH_3)_3$ | 5.85 | 74 |
| $CH_3SO_2CH_3$ | c. 23 | 74 |
| $CH(SO_2CH_3)_3$ | strong | 74 |
| $CH_2(CN)_2$ | 11.81 | 74 |
| $C_2H_5O_2CCH_2CN$ | 9 | 74 |
| $CH_3CO_2C_2H_5$ | ~ 24.5 | 74 |
| $CHC_2H_5(CO_2C_2H_5)_2$ | 15 | 74 |
| $CH_3CONH_2$ | ~ 25 | 74 |
|  | 6.10 | 74 |
|  | 10.96 | 74 |
|  | 7.82 | 74 |
| Dinitromethane | 4 | 2 |
| Potassium cyanide | 9.21 | 2 |
| $CH(CN)_3$ | strong | 74 |
| $CH_2(CO_2C_2H_5)_2$ | 13.3 | 74 |
| $CH_3CO_2H$ | ~ 24 | 74 |
|  | 10.5 | 74 |
|  | 10.1 | 74 |
| $CH_2(CHO)_2$ | 5 | 74 |

**Indicators**

| | | |
|---|---|---|
| Tropeoline OO | 2.0 | 28 |
| Bromocresol green | 4.9 | 28 |
| Thymol blue (1) | 1.65 | 28 |
| Methyl orange | 3.45 | 28 |
| Methyl yellow | 3.25 | 28 |
| Neutral red 7.4 | 28 | |
| Bromophenol blue | 4.1 | 28 |
| Bromothymol blue | 7.3 | 28 |
| Thymol blue (2) | 9.2 | 28 |
| Methyl red (1) | 2.3 | 28 |
| Methyl red (2) | 5.0 | 28 |

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