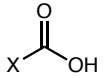
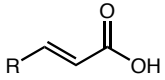
INORGANIC ACIDS

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	

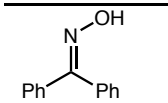


R= H	4.25	
trans-CO_2H	3.02, 4.38	
cis-CO_2H	1.92, 6.23	

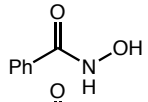
ALCOHOLS

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)

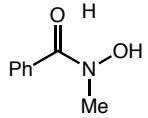
OXIMES & HYDROXAMIC ACIDS



11.3	(20.1)



8.88 (NH)	(13.7)

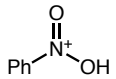


	(18.5)

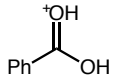
PEROXIDES

MeOOH	11.5
CH_3CO_3H	8.2

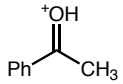
PROTONATED SPECIES



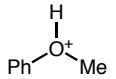
-12.4



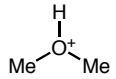
-7.8



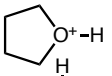
-6.2



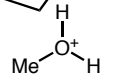
-6.5



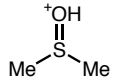
-3.8



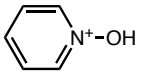
-2.05



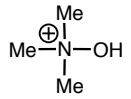
-2.2



-1.8

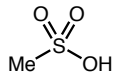


0.79	(+1.63)

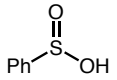


	(+5.55)

SULFINIC & SULFONIC ACIDS



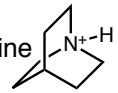
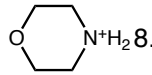
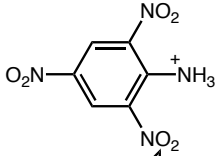
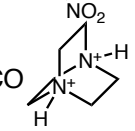
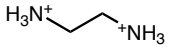
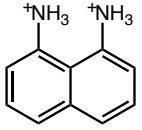
-2.6

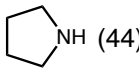
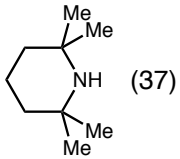
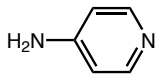
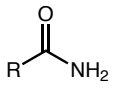
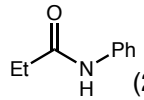
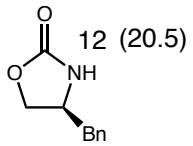
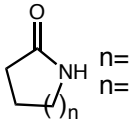
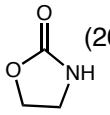
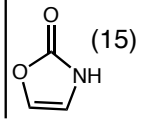
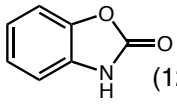


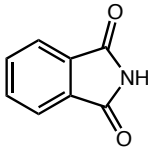
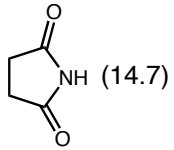
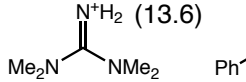
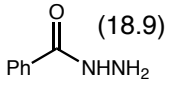
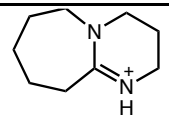
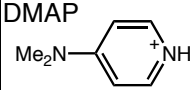
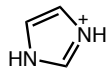
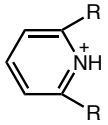
2.1

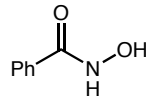
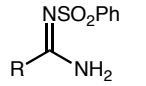
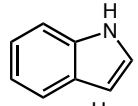
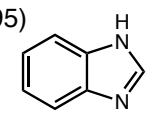
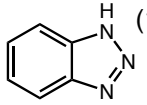
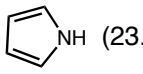
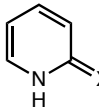
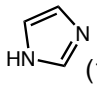
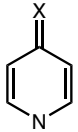
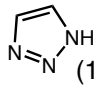
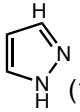
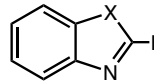
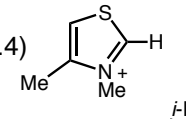
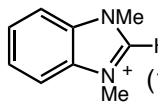
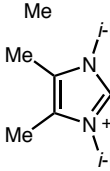
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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	

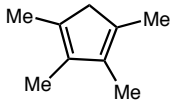
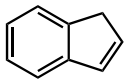
Substrate	pKa H_2O	(DMSO)
AMINES		
HN_3	4.7	(7.9)
NH_3	38	(41)
i-Pr_2NH	(36 THF))	
TMS_2NH	26(THF)	(30)
$PhNH_2$ (30.6)		
Ph_2NH (25.0)		
$NCNH_2$ (16.9)		
	(44)	
	(37)	
	(26.5)	
AMIDES & CARBAMATES		
	R= H	(23.5)
	CH_3 15.1	(25.5)
	Ph	(23.3)
	CF_3	(17.2)
	(urea) NH_2	(26.9)
	OEt	(24.8)
	(21.6)	
	12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

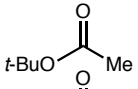
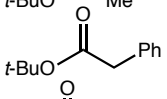
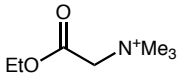
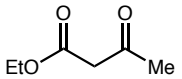
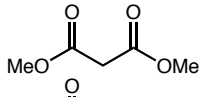
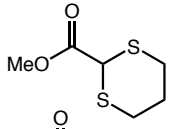
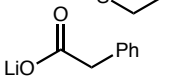
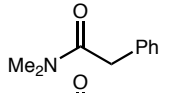
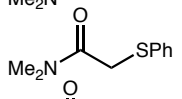
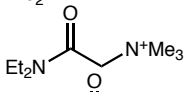
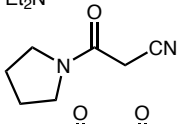
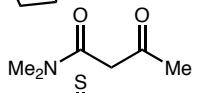
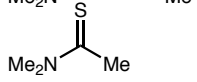
Substrate	pKa H_2O	(DMSO)
IMIDES		
	8.30	
		(14.7)
Ac_2NH		(17.9)
SULFONAMIDE		
RSO_2NH_2	R = Me	(17.5)
	Ph	(16.1)
	CF_3 6.3	(9.7)
$MeSO_2NHPh$		(12.9)
GUANIDINIUM, HYRDAZONES,- IDES, & -INES		
	N^+H_2 (13.6)	NNH_2 (21.6)
	(18.9)	
$PhSO_2NHNH_2$		(17.2)
PhNHNHPh		(26.1)
PROTONATED HETEROCYCLES		
DBU 	(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

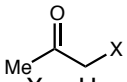
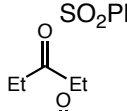
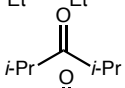
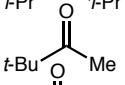
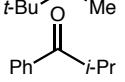
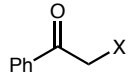
Substrate	pKa H_2O	(DMSO)
HYDROXAMIC ACID & AMIDINES		
	8.88 (NH)	(13.7)
	R= Me	(17.3)
	Ph	(15.0)
HETEROCYCLES		
	(20.95)	
	(16.4)	
	(11.9)	
	(23.0)	
	X= O (24) X= S (13.3)	
	(18.6)	
	X= O (14.8) X= S (11.8)	
	(13.9)	
	(19.8)	
	X= O (24.4) X= S (27.0)	
	(29.4)	
	(16.5)	
	(18.4)	
	(24)	

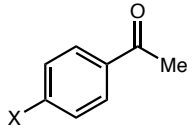
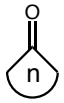
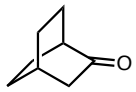
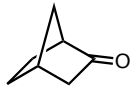
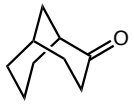
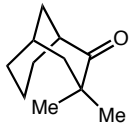
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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.

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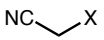
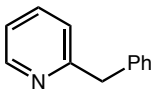
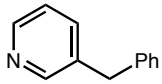
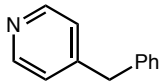
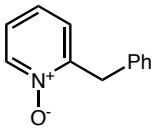
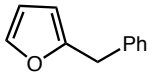
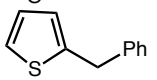
pKa's of CH bonds at Nitrile, Heteroaromatic, and Sulfur Substituted Carbon

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)

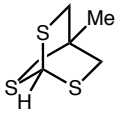
HETERO-AROMATICS

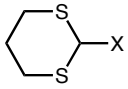
Substrate	pKa H_2O	(DMSO)
		(28.2)
		(30.1)
		(26.7)
		(25.2)
		(30.2)
		(30.0)

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)



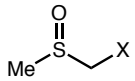
X=	Substrate	pKa H_2O	(DMSO)
	Ph		(30.7)
	CO_2Me		(20.8)
	CN		(19.1)

Substrate	pKa H_2O	(DMSO)
$RSCH_2CN$		

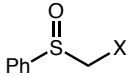
R=	Substrate	pKa H_2O	(DMSO)
	Me		(24.3)
	Et		(24.0)
	i-Pr		(23.6)
	t-Bu		(22.9)

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

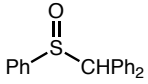
SULFOXIDES



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

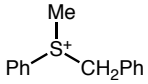


X=	Substrate	pKa H_2O	(DMSO)
	H		(33)
	Ph		(27.2)
	SOPh		(18.2)

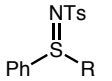


Substrate	pKa H_2O	(DMSO)
$Ph(CHPh_2)SO$		(24.5)

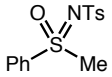
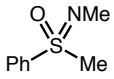
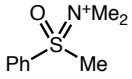
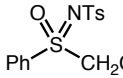
SULFONIUM

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

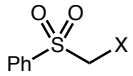
SULFIMIDES & SULFOXIMINES



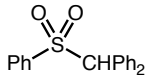
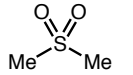
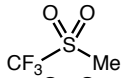
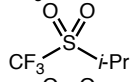
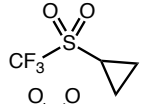
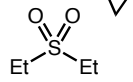
R=	Substrate	pKa H_2O	(DMSO)
	Me		(27.6)
	i-Pr		(30.7)

Substrate	pKa H_2O	(DMSO)
		(24.5)
		(33)
		(14.4)
		(20.7)

SULFONES

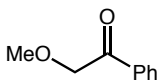
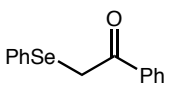


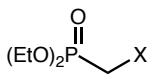
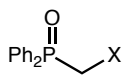
X=	Substrate	pKa H_2O	(DMSO)
	H		(29.0)
	CH_3		(31.0)
	t-Bu		(31.2)
	Ph		(23.4)
	$CH=CH_2$		(22.5)
	CH=CHPh		(20.2)
	CCH		(22.1)
	CCPh		(17.8)
	COPh		(11.4)
	COMe		(12.5)
	OPh		(27.9)
	N^+Me_3		(19.4)
	CN		(12.0)
	NO_2		(7.1)
	SMe		(23.5)
	SPh		(20.5)
	SO_2Ph		(12.2)
	PPh_2		(20.2)

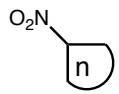
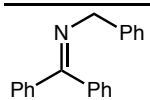
Substrate	pKa H_2O	(DMSO)
		(22.3)
		(31.1)
		(18.8)
		(21.8)
		(26.6)
		(32.8)
$(PhSO_2)_2CH_2Me$		(14.3)

*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

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JOC 41, 2786 (1976)
JOC 41, 2508 (1976)
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JOC 42, 326 (1977)
JOC 43, 3113 (1978)
JOC 43, 3095 (1978)
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J. March (1985)
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THF:
JACS 110, 5705 (1988)

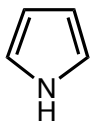
See cited website below for additional data

*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



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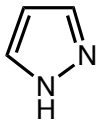

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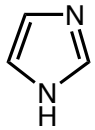

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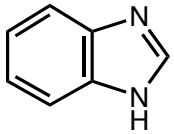

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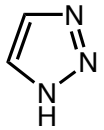

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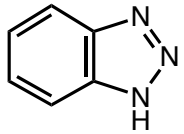

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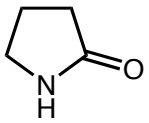

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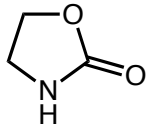

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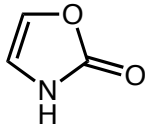

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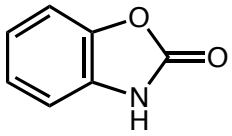

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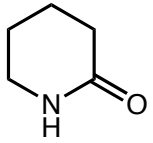

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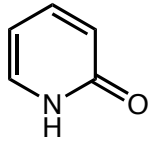

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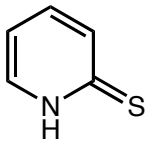

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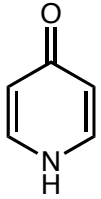

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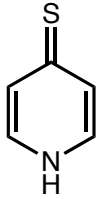

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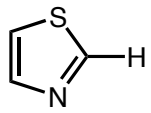

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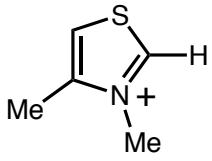

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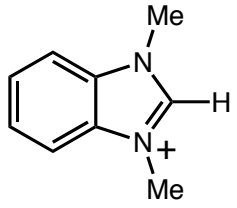

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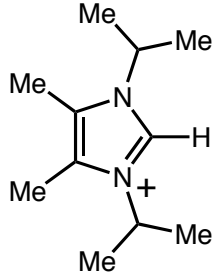

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pKa Values

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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

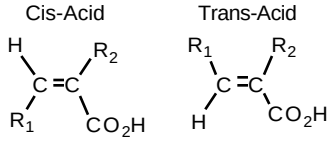
** Indicates thermodynamic values.*

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_5CH=$CHCO_2H$**	4.44*	2
$C_6H_5CH_2CH_2CO_2H$	4.66*	2
C_6H_5CH=$CHCO_2H$**	4.44	2
m-ClC_6H_4CH=$CHCO_2H$**	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
Δ^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

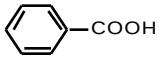
Hydroxycyclohexanecarboxylic acids

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-Δ^2-pyrroline	11.94	2
1-methyl-2-n-butyl-Δ^2-pyrroline	11.90	
1-Ethyl-2-methyl-Δ^2-pyrroline	11.92	2
1-n-Butyl-2-methyl-Δ^2-pyrroline	11.90	2
1,2-Dimethyl-Δ^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-Δ^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

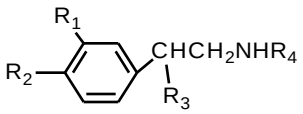
For complex chelating agents of aliphatic amines, see also ref. 77.

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)

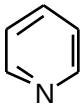
Unhindered	**pK**	**ref.**
Aniline	4.19	40
p-Aminodiphenyl	3.81	40
2-Naphthylamine	3.77	40
3-Phenanthrylamine	3.59	40
m-Aminodiphenyl	3.82	40
2-Aminofluorene	4.21	40
2-Phenanthrylamine	3.60	40
2-Anthrylamine	3.40	40
Hindered		
o-Aminodiphenyl	3.03	40
peri		
1-Naphthylamine	3.40	40
9-Phenanthrylamine	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

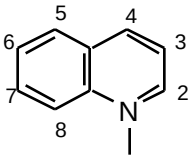
Nucleosides, etc.

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

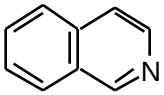
Heterocyclic Bases (Ref. 2)



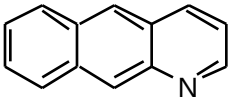
Pyridine 5.14*
pK (20°)



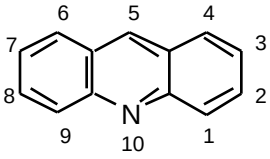
Quinoline 4.85*



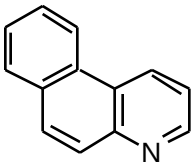
Isoquinoline 5.14*



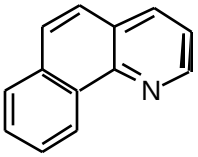
Benzoquinoline 5.05*



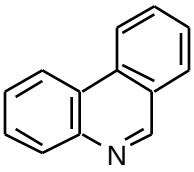
Acridine 5.60



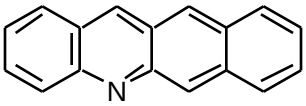
5,6-Benzoquinoline
5.15*



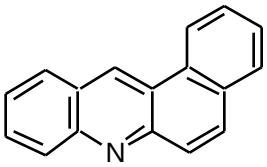
7,8-Benzoquinoline
4.25*



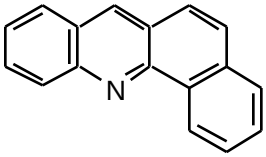
Phenanthridine 3.30[a]



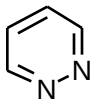
2,3-Benzacridine 4.52[a]



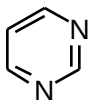
3,4-Benzacridine 4.70*



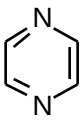
1,2-Benzacridine 3.45[a]



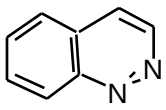
Pyridazine 2.10*



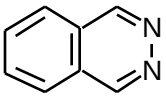
Pyrimidine 1.10*



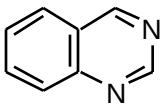
Pyrazine 0.37*



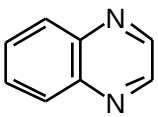
Cinnoline 2.64*



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_2Et	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_2Et	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-Δ^2-oxazoline	5.5
4-Carbamoyl-2-phenyl-Δ^2-oxazoline	2.9
2-Phenyl-Δ^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)

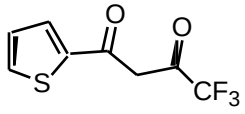
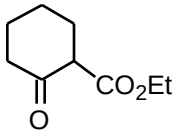
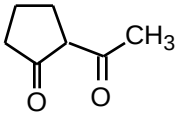
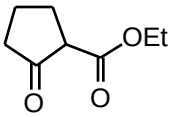
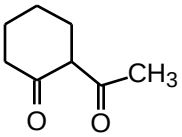
R	**R'**	**R"**	**pK**	**pK**
CH_3	CH_3	$(CH_2)_5CH_3$	11.33	12.52
CH_3	CH_3	C_6H_5	11.10	12.49
CH_3	CH_3	2-ClC_6H_4	11.04	12.73
CH_3	CH_3	2-C_5H_4N	9.80	12.46
CH_3	CH_3	2-$CH_3OC_6H_4$	11.47	12.44
CH_3	CH_3	3,4-$CH_2O_2C_6H_3$	11.39	12.60
CH_3	CH_3	3-C_5H_4N	10.29	12.63
CH_3	CH_3	4-$CH_3OC_6H_4$	11.62	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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