

pKa Values**INDEX**

Inorganic	2	Phenazine	24
Phosphates	3	Pyridine	25
Carboxylic acids	4, 8	Pyrazine	26
Aliphatic	4, 8		
Aromatic	7, 8	Quinoline	27
Phenols	9	Quinazoline	27
Alcohols and oxygen acids	10, 11	Quinoxaline	27
Amino Acids	12	Special Nitrogen Compounds	28
Peptides	13	Hydroxylamines	28
Nitrogen Compounds	14	Hydrazines	28
Aliphatic amines	15, 17, 19	Semicarbazones	28
Cyanoamines	16	Amidoximes	28
Anilines	17, 18, 20	Thiols	29
Nucleosides	21	Carbon Acids	30,31
Special Table Heterocycles	22	Indicators	31
Acridine	23	References	32-34
Benzoquinoline	24		
Cinnoline	23		
Hydantoin	24		
Imidazole	24		

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.			
			H ₃ PO ₂	2.0, 2.23*	28
			H ₂ PO ₄ ⁻	7.21*	77
AgOH	3.96	4	HPO ₄ ⁻	12.32*	77
Al(OH) ₃	11.2	28	H ₃ PO ₃	2.0	28
As(OH) ₃	9.22	28	H ₂ PO ₃ ⁻	6.58*	77
H ₃ AsO ₄	2.22, 7.0, 13.0	28	H ₄ P ₂ O ₇	1.52*	77
H ₂ AsO ₄ ⁻	6.98*	77	H ₃ P ₂ O ₇ ⁻	2.36*	77
HAsO ₄ [*]	11.53*	77	H ₂ P ₂ O ₇ ⁼	6.60*	77
As ₂ O ₃	0	4	HP ₂ O ₇ ⁼	9.25*	77
H ₃ AsO ₃	9.22*		HReO ₄	-1.25	30
H ₃ BO ₃	9.23*	28	HSCN	4.00	34
H ₂ B ₄ O ₇	4.00	34	H ₂ SeO ₃	2.6, 8.3, 2.62*	28
HB ₄ O ₇	9.00	34	HSeO ₃	8.32	77
Be(OH) ₂	3.7	4	H ₂ SeO ₄	Strong, 2.0	28
HBr	-9.00	31	HSeO ₄	2.00	34
HOBr	8.7	28	H ₃ SiO ₃	10.0	34
HOCl	7.53, 7.46	28, 33	H ₂ SO ₃	1.9, 7.0, 1.76*	28, 77
HClO ₂	2.0	28	H ₂ SO ₄	-3.0, 1.9	28
HClO ₃	-1.00	28	HSO ₃	7.21*	77
HClO ₄ (70%)	-10.00	31	HSO ₄ ⁻	1.99*	77
CH ₃ SO ₃ H	-0.6	31	H ₂ S ₂ O ₄	1.9	29
HCN	9.40	34	H ₂ Se	3.89*	77
H ₂ CO ₃	6.37, 6.35*, 3.58	34, 32	HSe ⁻	11.00*	77
HCO ₃	10.33*		H ₂ S	7.00*	77
H ₂ CrO ₄	-0.98	30	HS ⁻	12.92*	77
HCrO ₄	6.50*	2, 30	HSbO ₂	11.0	34
HOCN	3.92	34	HTe	5.00	34
HZ	3.17*, 0.59*	77	H ₂ Te	2.64, 11.0	34, 78
H ₂ GeO ₃	8.59, 12.72	34, 78	H ₂ TeO ₃	2.7, 8.0	28
Ge(OH) ₄	8.68, 12.7	28	Te(OH) ₆	6.2, 8.8	28
HI	-10.0	31	H ₂ VO ₄ ⁻	8.95	30
HOI	11.0	28	HVO ₄ ⁼	14.4	30
HIO ₃	0.8	28	H ₂ CrO ₄	0.74	77
H ₄ IO ₆ ⁻	6.00	34	HOCN	3.73	77
H ₅ IO ₆	1.64, 1.55, 8.27	34, 28	HSCN	0.85	77
HMnO ₄	-2.25	30	H ₃ PO ₂	1.07	77
NH ₃ OH [*]	5.98*		H ₃ PO ₄	2.12*	77
NH ₄ [*]	9.24*	77	H ₂ S ₂ O ₃	0.60*, 1.72*	77
HN ₃	4.72*	77	H ₃ AuO ₃	13.3, 16.0	78
HNO ₂	3.29	28	H ₃ GaO ₃	10.32, 11.7	78
HNO ₃	-1.3	28	H ₅ IO ₆	3.29, 6.70, 15.0	78
N ₂ H ₅ ⁺	7.99*	77		(see above!)	
H ₂ N ₂ O ₂	7.05	34	H ₄ V ₆ O ₁₇	1.96	78
H ₂ N ₂ O ₂ ⁻	11.0	34	H ₂ NSO ₃ H	1.0	80
H ₂ OsO ₅	12.1	34			
H ₂ O	15.7	none			
H ₃ O ⁺	-1.7	none			
Pb(OH) ₂	6.48 (10.92)	4 (78)			

* 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
-glycero-	1.40, 6.44	54
-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 ₂ O ₃ P(CH ₂) ₄ PO ₃ H ₂	<2, 2.75, 7.54, 8.38	57
H ₂ O ₃ P(CH ₂) ₃ PO ₃ H ₂	<2, 2.65, 7.34, 8.35	57
H ₂ O ₃ PCH ₂ CH(CH ₃)PO ₃ H ₂	<2, 2.6, 7.00, 9.27	57
H ₂ O ₃ PCH ₂ PO ₃ H 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) ₅ CH(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) ₂ NH ⁺ CH ₂ ⁻	--, 5.57	57
CHCl ₂ -	1.14, 5.61	57
CH ₂ Cl-	1.40, 6.30	57
CH ₂ Br-	1.14, 6.52	57
(-OOCCH ₂) ₂ NH ⁺ (CH ₂) ₂ -	--, 6.54	57
CH ₂ I-	1.30, 6.72	57
NH ₃ ⁺ CH ₂ CH ₂ -	2.45, 7.00	57
C ₆ H ₅ CH=CH-	2.00, 7.1	57
HOCH ₂ -	1.91, 7.15	57
C ₆ H ₅ NH ₂ ⁺ (CH ₂) ₃ ⁻	2.1, --	57
C ₆ H ₅ NH(CH ₂) ₃ ⁻	--, 7.17	57
Br(CH ₂) ₂ -	2.25, 7.3	57
CH ₃ (CH ₂) ₅ CH(COO ⁻)-	--, 7.5	57
C ₆ H ₅ CH 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) ₃ SiCH ₂ -	3.22, 8.70	57
C ₆ H ₅ CH ₂ -	3.3, 8.4	57
(C ₆ H ₅)SC-	3.85, 9.00	57

Arylphosphonic acids

2X-RC ₆ H ₃ PO ₃ H ₂			
X	R		
Cl	4-O ₂ N	1.12, 6.14	57
Br	5-O ₂ N	(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 ₃ O	4-O ₂ N	1.53, 6.96	57
CH ₃ O	H	2.16, 7.77	57
CH ₃ O	4-O ₂ N	--, 8.22	57
HO	4-O ₂ N	1.22, 5.39	57
O ₂ N	H	1.45, 6.74	57
F	H	1.64, 6.80	57
I	H	1.74, 7.06	57
NH ₂ H	--, 7.29	57	
CH ₃ H	2.10, 7.68	57	
C ₆ H 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 ₃ H ₂	2.35	7.1	1.85	5.35
X(CH ₂) ₂ PO ₃ H ₂	2.45	7.85	2.45	7.00
X(CH ₂) ₄ PO ₃ H ₂			2.55	7.55
X(CH ₂) ₅ PO ₃ H ₂			2.6	7.65
X(CH ₂) ₆ PO ₂ H ₂	2.6	7.9		
X(CH ₂) ₁₀ PO ₂ H 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
-keto- -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

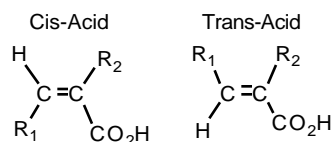
H-	4.76*	20
O ₂ N-	1.68*	20
(CH ₃) ₃ N ⁺ -	1.83*	20
(CH ₃) ₂ NH ⁺ -	1.95*	20
CH ₃ NH ₂ ⁺ -	2.16*	20
NH ₃ ⁺ -	2.31*	20
CH ₃ SO ₂ ⁻	2.36*	20
NC-	2.43*	20
C ₆ H ₅ SO ₂ ⁻	2.44	20
HO ₂ C	2.83*	20
C ₆ H ₅ SO-	2.66	20
F-	2.66	20
Cl-	2.86*	20
Br-	2.86	20
Cl ₂ ⁻	1.29	20
F ₂ ⁻	1.24	20
Br ₃ ⁻	0.66	20
Cl ₃ ⁻	0.65	20
F ₃ ⁻	0.23 (-0.26) (2)	20
HONC ₄	3.01	20
F ₃ C-	3.07*	20
N ₃ ⁻	3.03	20
I-	3.12	20
C ₆ H ₅ O-	3.12	20
C ₂ H ₅ O ₂ C-	3.35	20
C ₆ H ₅ S-	3.52*	20
CH ₃ O-	3.53	20
NCS-	3.58	20
CH ₃ CO-	3.58*	20
C ₂ H ₅ O-	3.60	20
n-C ₃ H ₇ O	3.65	20
n-C ₄ H ₉ O	3.66	20
sec.-C ₄ H ₉ O-	3.67	20
HS-	3.67*	20
i-C ₃ H ₇ O-	3.69*	20
CH ₃ S-	3.72*	20
i-C ₃ H ₇ S-	3.72*	20
C ₆ H ₅ CH ₂ S-	3.73*	20
C ₂ H ₅ S-	3.74*	20
n-C ₃ H ₇ S-	3.77*	20
n-C ₄ H ₉ S-	3.81*	20
HO-	3.83*	20
-O ₃ S-	4.05	20
(C ₆ H ₅) ₃ CS-	4.30*	20
C ₆ H ₅ -	4.31*	20
CH ₂ -CH-	4.35*	20

* Indicates thermodynamic values.

Unsaturated acids (25°)

Compound	pK	ref.	Compound	pK	ref.
trans-CH ₃ -CH=CHCO ₂ H	4.69*	20	H-CH ₂ CH ₂ CO ₂ H	4.88*	2
cis-CH ₃ -CH=CHCO ₂ H	4.44*	2	H-CH=CHCO ₂ H	4.25*	2
C ₆ H ₅ -CH ₂ CH ₂ CO ₂ H	4.66*	2	C ₆ H ₅ CH ₂ CH ₂ CO ₂ H	4.66*	2
trans-C ₆ H ₅ -CH=CHCO ₂ H	4.44*	2	C ₆ H ₅ CH=CHCO ₂ H**	4.44*	2
m-CH ₃ OC ₆ H ₄ CH ₂ CH ₂ CO ₂ H	4.65*		C ₆ H ₅ CH ₂ CH ₂ CO ₂ H	4.66*	2
	2		C ₆ H ₅ CH=CHCO ₂ H**	4.44	2
m-CH ₃ OC ₆ H ₄ CH=CHCO ₂ H	4.38*	2	m-ClC ₆ H ₄ CH=CHCO ₂ H**	4.29*	2
m-ClC ₆ H ₄ CH ₂ CH ₂ CO ₂ H	4.58*	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 ₆ H ₅ -	H-	3.88*	4.44*	2
ClC ₆ H ₄	H-	3.91	4.41	2
6-BrC ₆ H ₄	H-	4.02	4.41	2
CH ₃ -	CH ₃ -	4.30	5.02	2
C ₆ H ₅ -	H-	5.26***	5.58***	2
2,4,6-(CH ₃) ₃ C ₆ H ₂ -	H-	6.12***	5.70***	2
C ₆ H 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
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-2,3-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-Cyclopentane-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-cis-Cyclohexane-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- (high melting)	3.77, 5.94	2
Methyl-	3.05, 5.76	2	O-O'-Dimethyl- (low melting)	3.94, 6.20	2
Ethyl-	2.99, 5.83	2	O,O'-Diethyl- (high melting)	3.63, 6.46	2
n-propyl	3.00, 5.84	2	O,O'-Diethyl- (low melting)	3.51, 6.60	2
i-propyl-	2.94, 5.88	2	Tetramethyl-	3.50, 7.28	2
Dimethyl-	3.17, 6.06	2	Adipic	4.42, 5.41	2
Methylethyl-	2.86, 6.41	2	Pimelic	4.48, 5.42	2
Diethyl-	2.21, 7.29	2	Suberic	4.52, 5.40	2
Ethyl-n-propyl-	2.15, 7.43	2	Azelaic	4.55, 5.41	2
Di-n-propyl-	2.07, 7.51	2	DL-1:2-Dichlorosuccinic	1.68, 3.18	20
Glutaric	4.34, 5.42	2	meso-1:2-Dichlorosuccinic	1.74, 3.24	20
B-Methyl	4.25, 6.22	2	DL-1:2-Dibromosuccinic	1.48, ----	20
B-Ethyl	4.29, 6.33	2	meso-1:2-Dibromosuccinic	1.42, 2.97	20
B-n-Propyl	4.31, 6.39	2	DL-1:2-Dimethylsuccinic	3.93, 6.00	20
B,B-Dimethyl-	3.70, 6.29	2	meso-1:2-Dimethylsuccinic	3.77, 5.36	20
B,B-Methylethyl-	3.62, 6.70	2			
B,B-Diethyl-	3.62, 7.12	2			
B,B-Di-n-propyl	3.69, 7.31	2			
D-Tartaric	3.03, 4.45	20			
DL-Tartaric	3.03, ----	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	HO-	6.33	2
C ₂ H ₅ O ₂ C-	6.31	2	Br-	6.08	2
NC-	5.90	2	Lysergic acid, etc.		
			ergometrine	6.8, --	2
			Dihydroergometrine	7.4, --	2
			-dihydrolysergol	8.2, --	2

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

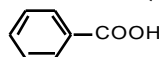
Hydroxycyclohexanecarboxylic acids

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 ₃ H	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 ₂ N-	2.17*	3.45*	3.44
CH ₃ CO-			
CH ₃ SO ₂ -		3.64*	3.52*
CH ₃ S-			
HS-			
Br-	2.85*	3.81*	4.00*
F-	3.27*	3.87*	4.14*
CH ₃ O-	4.09*	4.09*	4.47*
n-C ₃ H ₇ O-	4.24*	4.20*	4.46*
n-C ₄ H ₉ O-		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 ₆ H ₅ O-	3.53*	3.95*	4.52*
CH ₃ -	3.91*	4.24*	4.34*
(CH ₃) ₂ CH-			4.35*
(CH ₃) ₃ N ⁺ -	1.37	3.45	3.43
NC-		3.60*	3.55*
HO ₂ C*	2.95*	3.54	3.51
F ₃ C-		3.79	
HO-	2.98*	4.08*	4.58*
I-	2.85*	3.86*	
Cl-	2.94*	3.83*	3.99*
(CH ₃) ₃ Si-		4.24*	4.27*
C ₂ H ₅ O-	4.21*	4.17*	4.45*
i-C ₃ H ₇ O-	4.24*	4.15*	4.68*
n-C ₅ H ₁₁ O-			4.55*
C ₆ H ₅ -	3.46*		
CH ₃ CH ₂ -	3.77		4.35*
(CH ₃) ₃ C-	3.46	4.28	4.40*
-HO ₃ P-	3.78	4.03	3.95
-O ₃ S-		4.15	4.11
H ₂ N-	4.98	4.79	4.92
(CH ₃) ₂ N-	8.42	5.10	5.03
-HO ₃ As-			4.22
-O ₂ C-	5.41**	4.60	4.82
CH ₃ NH-	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 ₄ H 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 ₂ H ₅ -	3.77	2
2-C ₆ H 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*
						2.2, 8.96
						2.1, 8.91
						1.25, 4.14
						2.25, 10.03
						1.92, 2.28, 8.16
						2.97
						2.30, 6.60
						3.06, 4.34
						1.23, 6.69
						2.04, 10.47
						2.08, 9.80
						2.30, 10.10
						3.86
						4.39
						3.73
						2.98, 9.89
						4.04
						2.36, 10.06
						3.53
						2.24, 10.01
						3.03, 3.07, 10.
						1.95, 2.45, 6.54, 10.46

*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
-carboxymethylaminopropionic	3.61, 9.46
, -diaminobutyric	1.85, 8.24, 10.44
Di-(carboxymethyl)-aminomethyl phosphonic acid	2.00, 2.25, 5.57, 10.76
, -dimercaptosuccinic	2.40, 3.46, 9.44, 11.82
Ethylenediamine-N,N-diacetic	5.58, 11.05
-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

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-Hydroxybenzaldehyde	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 ₂ N-	7.23*	8.35*	7.14*	
(CH ₃) ₃ N ⁺ -	7.42	8	8		OCH-	6.79	8.00	7.66	
CH ₃ SO ₂ -		9.33	7.83		NC-		8.61**	7.95	
CH ₃ CO-		9.19	8.05		CH ₃ O ₂ C-			8.47*	
C ₂ H ₅ O ₂ C-			8.50*		n-C ₄ H ₉ O ₂ C-			8.47*	
C ₃ H ₅ CH ₂ O ₂ C-			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 ₃ S-		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 ₂ H ₅ -	10.2	9.9	10.0	
CH ₃ O-	9.93	9.65	10.20		H ₂ N-	9.71	9.87	10.30	
-O ₂ C-		9.94*	9.39*		-O ₃ S-		9.29	9.03	
--O ₃ P-		10.2	9.9		--O ₃ As				8.37
C ₆ H 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.	Compound	pK	Ref.
Choline	13.9	6	C ₃ F ₇ •CH(C ₂ F ₅)•OH	10.48	65
Chloral hydrate	9.66, 11.0	61	(C ₃ F ₇) ₂ CH•OH	10.52	65
Trifluoroethanol	11.4, 12.43	63	62 Carbonium ions		
CF ₃ CH ₂ OH	11.8	63	Triphenylmethanols in		
CF ₃ CH(OH)CH ₃	12.43	10	4,4,4-Trimethoxy	H ₂ SO ₄ .82, HClO ₄ .82, HNO ₃ .82	ref .80 66
CF ₃ CH ₂ (CH ₃) ₃ OH	11.4**	63	4,4'-Dimethoxy	-1.24	-1.14 -1.11 66
(C ₃ F ₇) ₂ CHOH	10.6**	63	4-Methoxy	-3.40	-3.59 -3.41 66
HCCCH ₂ OH	13.55	64	4-Methyl	-5.41	-5.67 66
C(CH ₂ OH) ₄	14.1	64	4-Trideuteriomethyl-	5.43	5.67 66
HOCH ₂ CHOHCH ₂ OH	4.4	64	3,3',3''-Trimethyl-	6.35	-5.95 66
HOCH ₂ CH ₂ OH	14.77	64	Unsubstituted triphenyl-		
CH ₃ CCH ₂ OH	14.82	64	methanol-	6.63	-6.89 6.60 66
CH ₃ OH	15.54		64 4,4,4;-Trichloro-		7.74- 8.01 66
CH ₂ =CHCH ₂ OH	15.52		64 4-Nitro-		9.15- 9.76 66
H ₂ O	15.74	64	CCl ₃ CH ₂ OH	11.8***	
CH ₃ CH ₂ OH	16	64	CF ₃ CH ₂ OH	11.3***	
Substituent effects for ionization of RCH₂OH					
R					
CCl-3	12.24,11.80	64,65			
CF ₃ -	12.37	64			
CHF ₂ CH ₂ -	12.74	64	Hydroxamic acids		
CHCl ₂ -	12.89	64	Furo-	8.45	72
CHEC-	13.55	64	Glycine	7.40	72
H ₂ Cl-	14.31	64	Hippuro-	8.80	72
CH ₃ CCH ₂ -	14.8	64	isoNicotin	7.85	72
HOCH ₂	15.1		64 p-Methylbenz-		8.90 72
H-	15.5	64	Nicotin-		8.30 72
CH ₂ =CH-	15.5	64	Nicotin-methiodide	6.46	72
CH ₃ -(extrap)	(15.9)	64	m-Nitrobenz-	8.07	72
CF ₃ C(CH ₃) ₂ OH	11.6	64	Picolin	8.50	72
HOCH ₂ CF ₂ CH ₂ OH	11	64	Pyrimidine-2-carbox-	7.88	72
Primary alcohols=R•CH ₂ •OH and			Salicyl-	7.43	72
Secondary alcohols in 50% alcohol			Tropo-		9.09 72
C ₂ F ₅	11.35	65			
C ₄ F ₉	11.35	65			
C ₅ F ₁₁	11.37	65			
C ₇ F ₁₅	11.35	65	Other oxygen acids		
CHF ₂	12.00	65	Trimethylamine-n-oxide	4.6	18
CF ₂ Cl	11.63	65	Dimethylglyoxime		12.84 77
CHF ₂ CF ₂	11.34	65	(50% dioxane)		
CHF ₂ •(CF ₂) ₂	11.35	65	O-methyl ether	12.92	77
CF ₃ •CH ₂	12.7	65	Tropolone	12a	77
CF ₃ •(CH ₂) ₂	12.9	65	-Bromotropolone	6.95 ^a	77
CF ₃ •CHMe•OH	11.28	65	Acetald hydrate	13.48	91
C ₃ F ₇ •CHMe•OH	11.38	65	Formald hydrate	13.29	91
C ₃ F ₇ CH ₂ Et•OH	11.37	65			
C ₃ F ₇ CH ₂ Pr•OH	11.37	65			
C ₃ F ₇ •CH(CF ₃)•OH	10.46	65			

^a50% dioxane
 ***50 aqueous 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-Benzyloxy pyridine 1-oxide	1.99	67
1-Benzyloxy pyrid-4-one	2.58	67
2-Methoxypyridine 1-oxide	1.23	67
1-Benzyloxy pyrid-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 ₄ H 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 ₂ H ₅	iso-C ₃ H ₇	tert-C ₄ H ₉	iso-C ₄ H 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

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
-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-Cyclohexanetrionetrixime	8.0	76
5-Methyl-1,2,3-cyclohexane-trionetrixime	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

Pyridine-2-aldoxime heptiodide	8.00
Pyridine-4-aldoxime methiodide	8.50
Pyridine-4-aldoxime pentiodide	8.50

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	pK		Ref.
Compound	-COOH		-NH₃
Alanine	2.35	9.69	6
-Aminobutyric acid	2.55	9.60	
-Aminoisobutyric	2.36	10.21	6
Argininosuccinic	>12, 1.62	9.58	6
	2.70, 4.26		
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		9.17
	6		
Hydroxylsine	2.13	8.62	6
		9.67	
Isoleucine	2.36	9.68	6
Lysine	2.18	8.95	6
		10.53	
O-Methyl tyrosine		9.27	21

O-Methyltyrosine ethyl ester	7.31		22	
octopine	13, 1.36		8.77	
	6			
	2.40			
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	
-Alanine	3.60	10.19	6	
-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	8.68		6
	11.68			
Glutamine		2.17	9.13	6
Histamine	5.0		9.7	6
-Hydroxyglutamic acid		2.09	9.20	6
		4.18		
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	6
			10.76	
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	6.36	6
		3.12	6.95	
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		

Lysyllsine (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				Trimethylsilylmethyl-	10.96	1	
-Alanine ester	9.13	1		CH ₃ ONH ₂	4.60	12	
Allylamine-	9.69	2		Allyl-	9.49	1	
Benzyl	9.34	1		-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		-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		-Phenylbutyl	10.40	2	
-Phenylethyl-	9.83	1		-Phenylpropyl-	10.20	1	
				Triethylenedi-	8.8*	?	
X	XNH₃⁺	XCH₂NH₃⁺	X(CH₂)₂NH₃⁺	X(CH₂)₃NH₃⁺	X(CH₂)₄NH₃⁺	X(CH₂)₅NH₃⁺	ref.
H-	9.25*	10.64*	10.67*	10.58*	10.61*	10.63*	2
HF ₂ C-		7.52					
RO ₂ C-		7.75	9.13	9.71	10.15*	10.37	2
HO-	5.96*		9.50*				
C ₆ H ₅ -	4.58*	9.37*	9.83*	10.20*	10.39*	10.49*	2
H ₂ N-	8.12*		9.98*	10.65*	10.84*	11.05*	2
H ₂ C=CH-		9.69					
CH ₃ -	10.64*	10.67*	10.58*	10.61*	10.63*	10.64*	2
X	-H	-NH₃⁺	-CO₂⁻	-SO₃⁻	-PO₃⁻		2
X-NH ₃ ⁺	9.25*	-.88		1	10.25		
X(CH ₂) ₂ NH ₃ ⁺	10.64			9.77	5.75	10.8	
X(CH ₂) ₂ NH ₃ ⁺	10.67			10.19	9.20	10.8	
X(CH ₂) ₄ NH ₃ ⁺	10.61	9.31		10.77	10.65	10.9	
X(CH ₂) ₅ NH ₃ ⁺	10.63	9.74		10.75	10.95	11.0	
X(CH ₂) ₈ NH ₃ ⁺	10.65	10.10					
X(CH ₂) ₁₀ NH ₃ ⁺	10.64				11.35	11.25	
X(CH ₂) ₃ NH ₃ ⁺	10.58	8.59		10.43	10.05		
Secondary amines				Di-n-butyl-	11.25	1	
Dimethyl-	10.64	1		Diisobutyl-	10.50	1	
Di-n-propyl-	11.00	1		-Ethylpyrroline	7.43	2	
Diisopropyl-	11.05	1		-Benzylpyrroline-	7.08	2	
t-Butylcyclohexyl-	11.23	1		2-Methylpiperidine	10.99	2	
-Cyclohexylpyrroline	7.95	2		-Cyclohexylpyrrolidine	10.80	2	
-(p-Tolyl)pyrroline	7.59	2		-(p-Tolyl)pyrrolidine	10.01	2	
-Ethylpyrrolidine	10.43	2		N,O-dimethylhydroxylamine	4.75	12	
-Benzylpyrrolidine	10.36	2		Acetanilide	+0.61	4	
N-methylhydroxylamine	5.96	12		<i>*thermodynamic value</i>			
Diethyl-	10.98	1					

Aliphatic Amines			Methyl- -diethylamino-ethyl-sulfide		
1,2-Iminoethane	7.98	7	1,2-Dimethyl- 2-pyrroline	11.94	2
cis-2,3-Iminobutane	8.72	7	1-methyl-2-n-butyl- 2-pyrroline	11.90	
1,2-Imino-2-methylpropane	8.61	7	1-Ethyl-2-methyl- 2-pyrroline	11.92	2
1,2-Iminobutane	8.29	7	1-n-Butyl-2-methyl- 2-pyrroline	11.90	2
trans-2,3-Iminobutane	8.69	7	1,2-Dimethyl- 2-tetrahydropyridine	11.57	2
Secondary Amines			N-Ethyl derivative of: 1,2-Imino-ethane		
Allylmethyl-	10.11	1		7.93	7
Benzylethyl-	9.68	1	Trans-2,3-Iminobutane	9.47	7
Morpholine	8.36	1	Trimethylhydroxylamine	3.65	12
N-Benzoylpiperazine	7.78	1	Dimethylethyl-	9.99	1
Di-sec-butyl-	11.01	1	Triethyl-	10.65	1
N-Methylmethoxyamine	4.75	1	Dimethyl-n-butyl-	10.02	1
Pyrolidine	11.27	1	Dimethyl-isopropyl-	10.30	1
1-Tosylpiperazine	7.39		Dimethyl-t-butyl-	10.52	1
Benzylmethyl-	9.58	1	Tri-n-butyl-	10.89	1
Piperidine	11.22	1	Diallylmethyl-	8.79	1
N-Carbethoxypiperazin	8.28	1	1-n-Propylpiperidine	10.48	2
Dietrimethylsilylmethyl-	11.40	1	10.1	10.1	5
Diallyl-	9.29	1	9.8	--	5
N-Methylhydroxyl-	5.96	1	1,2-Dimethylpyrrolidine	10.26	2
Trimethyleneimine	11.29	1	1-Methyl-2-n-butylpyrrolidin	10.24	2
Cis-2,6-dimethyl-piperidine	10.92	3	1-Ethyl-2-methylpyrrolidine	10.64	2
Tertiary amines			1-n-Butyl-2-methylpyrrolidine		
Trimethyl-	9.76	1	1-Ethyl-2-methylpyrrolidine	10.70	2
Dimethyldiethyl-	10.29	1	1,2-Iminobutane	8.18	7
Dimethyl-n-propyl-	9.99	1	cis-2,3-Iminobutane	8.56	7
Dimethyl-isobutyl-	9.91	1	N-dimethylhydroxylamine	5.20	12
Dimethyl-sec-butyl-	10.40	1	Allyldimethyl	8.78	1
Tri-n-propyl-	10.65	1	1,2-Dimethylpiperidine	10.26	2
Triallyl-	8.31	1	1-Ethyl-2-methyl- 2-tetrahydropyridine	11.57	2
N-Allylpiperidine	9.69	2			
1-Diethylamino-hexane-thiol-(6)					
Cyanoamines			2-Amino-2-cyanopropane		
N-piperidine-CH ₂ CN	4.55	8	-Isopropylaminopropionitrile	8.0	9
Et ₂ NCN	-2.0	8	-Diethylaminopropionitrile	7.6	9
Et ₂ N(CH ₂) ₂ CN	7.65	8	Et ₂ NCH ₂ CN	4.55	8
Et ₂ N(CH ₂) ₄ CN	10.08	8	Et ₂ N(CH ₂) ₃ CN	9.29	8
Et ₂ NC(CH ₃) ₂ CN	9.13	8	Et ₂ N(CH ₂) ₅ CN	10.46	8
EtN(CH ₂ CN) ₂	-0.6	8	HN(CH ₂ CN) ₂	0.2	8
EtN(CH ₂ CH ₂ CN) ₂	4.55	8	HN(CH ₂ CH ₂ CN) ₂	5.26	8
H ₂ NCH ₂ CN	5.34	8	N(CH ₂ CH ₂ CN) ₃	1.1	8
N-Amphetamine-(CH ₂) ₂ -CN	7.23	8	N-piperidine-C(CH ₃) ₂ CN	9.22	8
N-Norcodeine-(CH ₂) ₂ CN	5.68	8	N-Methamphetamine-(CH ₂) ₂ CN	6.95	8
Dimethylcyanamide	1.2	9	Methyl cyanamide	1.2	9
Diethylcyanamide	1.2	9	Ethyl cyanamide	1.2	9
Aminoacetonitrile	5.3	9	Cyanamide	1.1	9
Diethylaminoacetonitrile	4.5	9	Dimethylaminoacetonitrile	4.2	9

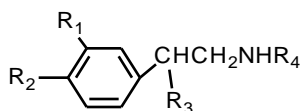
-Aminopropionitrile	7.7	9
-Dimethylaminopropionitrile	7.0	9
, "-Dicyanodiethylamine	5.2	9

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

Fluoro-substituted amines

CF ₃ CH ₂ NH ₂	5.7	10
CF ₃ CH ₂ N(CH ₃) ₂	4.75	10

CF ₃ CH ₂ NHCH 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	Cyclotridecyl	9.63
Hexamethylene	10.00	Cyclotetradecyl	9.54
Heptamethylene	9.77	Cyclopentadecyl	9.54
Octamethylene	9.39	Cycloheptadecyl	9.57
Nonamethylene	9.14	Cyclooctadecyl	9.54
Decamethylene	9.04		
Undecamethylene	9.14	Amines other	
Dodecamethylene	9.31	Dimeoone	5.23 18
Tridecamethylene	9.35	Phthalimide	8.30 18
Tetradecamethylene	9.35	Nitrourea	4.57 18
Hexadecamethylene	9.29	Nitrourethane	3.28 18
Heptadecamethylene	9.27	Diphenylthiocarbazone	4.5 6
Cyclohexyl	9.82	, , "-Triaminotriethylamine	8.42, 9.44, 10.13 87
Cycloheptyl	9.99		
Cyclooctyl			
Cyclononyl	9.95	Anilines	Ref. 2
Cyclodecyl	9.85	Monosubstituted	
Cycloundecyl	9.71	Substituent	o m p
Cyclododecyl	9.62	H-	4.62* 4.64* 4.58*

(CH ₃) ₃ N ⁺ -		2.26	2.51	p-(CH ₃) ₃ C-	4.65
CH ₃ O ₂ C-	2.16	3.56	2.30	m-Br-	3.08
CH ₃ SO ₂ -		2.68*	1.48	m-Cl-	3.09
CH ₃ S-		4.05	4.40	p-F-	4.01
Br-	2.60*	3.51*	3.91*	p-(CH ₃) ₃ Si-	3.99
F-	2.96*	3.38*	4.52*	p-CH ₃ O-	5.14, 5.16
CH ₃ O-	4.49*	4.20*	5.29*		
C ₆ H ₅ -	3.78*	4.18	4.27*		
(CH ₃) ₃ C-	3.78				
-O ₃ S-		3.80	3.32		
H ₃ N ⁺	1.3	2.65	3.29		
O ₂ N-	-0.28*	2.45*	0.98*, 1.11*		
HO ₂ C-	2.04	3.05	2.32		
C ₂ H ₅ O ₂ C-	2.10		2.38		
F ₃ C-		3.49*	2.57*		
HO-	4.72	4.17	5.50		
Cl-	2.62*	3.32*	3.81*		
(CH ₃) ₃ Si-		4.64*	4.36*		
C ₂ H ₅ O-	4.47*	4.17*	5.25*		
CH ₃ -	4.38*	4.67*	5.07*		
-HO ₃ As	3.77	4.05	4.05		
H ₂ N-	4.47	4.88	6.08		

*Thermodynamic

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 XC₆H₄N(CH₃)₂ ref. 2

H-	4.21, 4.09
m-CH ₃	4.66
p-C ₂ H ₅ -	4.69
o-(CH ₃) ₂ CH-	5.05
p-CH ₃ CH ₂ CH ₂ CH ₂ -	4.62
o-(CH ₃) ₃ C-	4.26
p-I-	3.43, 2.73
p-Br-	3.52, 2.82
p-Cl-	3.33
m-(CH ₃) ₃ Si-	4.41
o-CH ₃ O-	5.49
o-CH ₃	5.15, 5.07
p-CH ₃	4.94
p-CH ₃ CH ₂ CH ₂ -	4.43
p-(CH ₃) ₂ CH-	4.77
p-(CH ₃) ₂ CHCH 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) ₂ CH-	4.06
2-(CH ₃) ₂ C-	3.38
2,6-(CH ₃) ₂ -4-(CH ₃) ₃ C-	3.88
2,4-(CH ₃) ₂ -6-(CH ₃) ₃ -	3.43
2-CH ₃ -4,6-(CH ₃) ₃ C-	3.31
2,4,6-[(CH ₃) ₃ C 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 ₆ H ₅ NHR	C ₆ H ₅ N(CH ₃)R	C ₆ H ₅ NR ₂	2-CH ₃ C ₆ H ₄ NHR	2-CH ₃ C ₆ H ₄ NR 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 ₂ H ₅ -	5.11	5.98	6.56	4.92	7.18
n-C ₃ H ₇ -	5.02	--	5.59	--	--
n-C ₄ H ₉ -	4.95	--	~5.7	--	--
i-C ₄ H ₉ -	--	5.20	--	--	--
sec-C ₄ H ₉ -	--	6.04	--	--	--
t-C ₆ H ₁₂ -	6.30	--	--	--	--
Cyclopentyl-	5.30	6.71	--	5.07	--
Cyclohexyl-	5.60	6.35	--	5.34	--
t-C ₄ H 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- -amino- -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
-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
Benzyl dimethyl	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
Benzyl diethyl	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			Methyl-[-diethylamino-ethyl]sulfide	9.8
N-Dimethyl-cysteamine	7.95, 10.7		N-Diethyl-cysteamine	7.8, 10.75
N-Dipropyl-cysteamine	8.00, 10.8		N- -Mercaptoethyl-piperidine	7.95, 11.05
N- -Mercaptoethyl-morpholine	6.65, 9.8		1-Diethylamino-propan- (3)	8.0, 10.5
1-Diethylamino-butan- (4)	10.1		1-Diethylamino-hexan- (6)	10.1

ANILINES (Ref. 88)

m-Substituted anilines

m-C ₂ H 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		

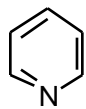
NAPHTHALAMINES (reference 88)

substituted naphthalamines

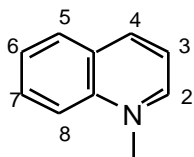
2-naphthalamine	X		2-naphthalamine	X	
1-NH ₂ ,3-X	NO ₂	2.07	2-NH ₂ ,4-X	NO ₂	2.43
	CN	2.26		CN	2.66
	Cl	2.66		Cl	3.38
	Br	2.67		Br	3.40
	I	2.82		I	3.41
	COOCH ₃	3.12		COOCH ₃	3.38
	OCH ₃	3.26		OCH ₃	4.05
	OH	3.30	1-NH ₂ ,6-X	NO ₂	2.89
	CH ₃	3.96		Cl	3.48
	Cl	2.71		OCH ₃	3.90
2-NH ₂ ,5-X	NO ₂	3.01		OH	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	10.40, 5.28	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			

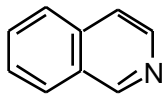
Heterocyclic Bases (Ref. 2)



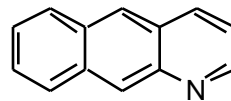
Pyridine 5.14*
pK (20°)



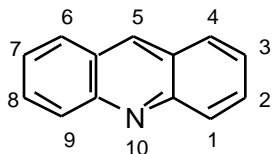
Quinoline 4.85*



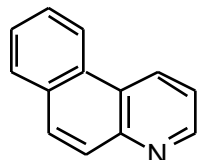
Isoquinoline 5.14*



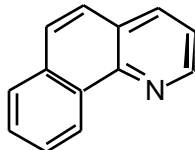
Benzoquinoline 5.05*



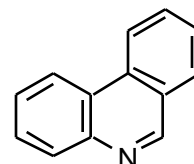
Acridine 5.60



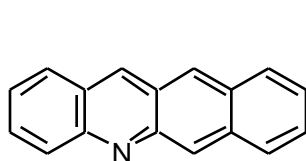
5,6-Benzoquinoline
5.15*



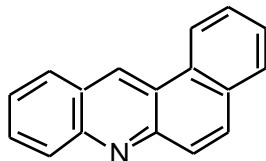
7,8-Benzoquinoline
4.25*



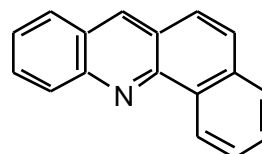
Phenanthridine 3.30^a



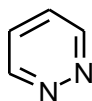
2,3-Benzacridine 4.52^a



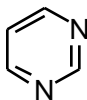
3,4-Benzacridine 4.70*



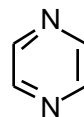
1,2-Benzacridine 3.45^a



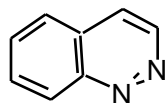
Pyridazine 2.10*



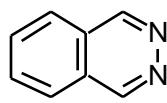
Pyrimidine 1.10*



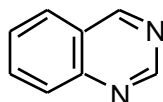
Pyrazine 0.37*



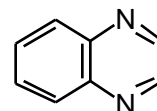
Cinnoline 2.64*



Phthalazine 3.39*



Quinazoline 3.31*



Quinoxaline 0.6*

^a 50% EtOH

Heterocyclics

Aureomycin

3.30, 7.44, 9.27

77

3-Hydroxy

8.81, 5.52

39

Iridine

--, 5.62

39

5-Hydroxy (acridone)

--f, -0.32

39

5-Methoxy

--, 7

39

Acridine

1--

2--

3--

4--

5--

9--

Ref. 2

H--	5.60*	4.11 ^a			
H ₂ N--	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 ₂ K-(1-CH ₃ --)--				4.79 ^a	9.73 ^s
1,9-(CH ₃) ₂ --	2.88 ^a				3.22 ^a

^a 50% ethanol; ref. 39

8-amino-1,2-benzacridine	6.72	40	, ' -dipyridyl	4.43	6
2-amino-4-methyl-5,6-benzoquinoline	7.14		4-amino-	8.75 ^a	19
	40		4-amino-2-methyl-	9.45 ^a	19
3-amino-6,7-benzoquinoline	4.78	40	4-amino-2-methyl-8-chloro-	5.95 ^a	19
8-amino-3,4-benzacridine	7.42	40	8-chloro-	2.5 ^a	19
1'-amino-5,6-benzoquinoline	5.03	40	3,4-diamino-	8.15 ^a	19
4'-amino-5,6-benzoquinoline	5.20	40	3-amino-	4.78, 3.73 ^a	19
2-amino-4-methyl-7,8,benzoquinoline			7,8-benzquinoline	4.25, 3.15 ^a	19
	6.74	40	4-amino-	7.68 ^a	19
6,7-benzoquinoline	5.05, 3.84 ^a	19	4-amino-2-methyl-	7.96 ^a	19
5,6-benzoquinoline	5.15, 3.90 ^a	19	2-amino-4-methyl-	6.74, 6.02 ^a	19
4-amino-	7.99 ^a	19	6-amino-2-methyl-	5.23 ^a	19
2-methyl-	4.44 ^a	19	1'-amino-2-methyl-	4.75 ^a	19
4-amino-2-methyl-	8.45 ^a	19	3,4-benzacridine	4.70, 4.16 ^a	19
2-amino-4-methyl-	7.14, 6.51 ^a	19	5-amino	8.41 ^a	19
4'-amino-	5.20, 4.10 ^a	19	7-amino-	5.03 ^a	19
3'-amino-	4.02 ^a	19	8-amino-	7.42 (6.51) ^a	19
1'-amino-	5.03	19	8-acetamido-	4.48 ^a	19
2',4'-diamino-	4.91 ^a	19	8-dimethylamino-	7.31, 6.99	19
Benziminazole	5.53	19	1,2-benzacridine	3.45 ^a	19
2-amino-	7.54	19	5-amino-	8.13 ^a	19
Benztriazole	1.6	19	7-amino	4.05 ^a	19
Benzthiazole	1.2, 0.1 ^a	19	8-amino-	6.72, 5.97 ^a	19
2-amino-	4.51	19	4',5'-diamino-	8.44 ^a	19
benzoxazole	(decomp.)	19	Cinnoline	--, 0.21	39
2-amino-	3.73	19	3-hydroxy	8.64, 0.21	39
2,3-benzacridine	4.52 ^a	19	5-hydroxy	7.40, 1.92	39
5-amino-	9.72 ^a	19	7-hydroxy	7.56, 3.31	39
5-acetamido-	4.56 ^a	19	4-methoxy	--, 3.21	39
7-amino-	5.38 ^a	19			
5-amino-6:7:8:9-tetrahydro-	9.66 ^a	19	Heterocyclics		
Caffeine	0.61	4	o,o'-dipyridyl	4.43	6
cinchonine	7.2	4	hydantoin	9.16	42
Cinnoline	2.70	19	5-isopropyl-2-thio-	8.70	42
4-amino-	6.84	19	5,5-pentamethylene2-thio	8.79	42
Cocaine	7.6	4	3,5,5-trimethyl-2-thio	10.80	42
Cinnoline 4-hydroxy	9.27, 0.35	39	3-methyl-5,5-pentamethylene-2-thio-	11.23	42
6-hydroxy	7.52, 3.65	39			
-hydroxy	8.20, 2.74	39	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
Picolinic 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-Methylacetamido)-	3.52	46
3-(N-Methylbenzamido)-	3.66	46
4-(N-Methylacetamido)-	4.62	46

4-(N-Methylbenzamido)-	4.68	46	(CH ₃) ₂ CH-	5.83 ^b	5.72 ^b	6.02 ^b
4-Benzamido-	5.32	46	CH ₃ CO		3.18 ^b	
3-NO ₂	0.81	88	H ₂ N-	6.68 ^b	5.80 ^b	8.96 ^b
3-COO ⁻	4.77	47	CONH ₂ ⁴⁷		3.40	3.61
2,3-Me ₂	6.60	48	NC- ⁴⁷		1.45	
2,5-Me ₂	6.47	48				
3,4-Me ₂	6.52	48				
2,4,6-Me ₃	7.48	48				
4-OEt	6.67	48				
3-Cl	2.84	48				
3-CO ₂ Et	3.35	48				
3-COOH	3.13	88				
2-Amyl-	6.00 ^b	45				
2-Hexyl-	5.95 ^b	45				
2-Benzyl-	5.13	45				
2-Bromo-	0.71	45				
2,4-Dihydroxy	6.50, 13, 1.37	39				
1-Methyl-2-pyridone	0.32	39				
2-Acetamido-	4.09	46				
1-Methylpyrid-2-one acetylimine	7.12	46				
3-Acetamido-	4.46	46				
3-Benzamido-	3.80	46				
1-Methylpyrid-4-one acetylimine						
	11.03	46				
1-Methylpyrid-4-one benzylimine	9.89	46				
4-COO ⁻	4.90	47				
2,4-Me ₂	6.72	48				
2,6-Me ₂	6.77	48				
3,5-Me ₂	6.14	48				
2-Me,5-Et	6.51	48				
3-F	3.10	48				
3-Br	2.84	48				
4-CO ₂ Et	3.45	48				

Pyridine N-oxides (see oxygen acids)

Substituted Pyridines

Pyridine	2-	3-	4-
H-	5.17 ^b		
Cl-	0.72 ^b	2.84 ^b	
I-	1.82 ^b	3.25 ^b	
CH ₃ CH ₂ -	5.97 ^b	5.70 ^b	6.02 ^b
(CH ₃) ₃ C-	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 ₃ O-	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

Ortho-Substituted Pyridines (in 50% ethanol)

Substituent	pK	ref.
H-	4.38	2
2-C ₂ H ₅ -	4.93	2
2-(CH ₃)	4.68	2
2,6-[(CH ₃) ₂ CH] ₂	3.58	2
2-(CH ₃) ₃ C-	4.68	2
2-C ₂ H ₅ -6-(CH ₃) ₃ C-	4.36	2
2,6-[(CH ₃) ₃ C] ₂ ⁻	3.58	2
2-CH ₃ -	5.05	2
2-(CH ₃) ₂ CH-	4.82	2
2,6-(CH ₃) ₂	5.77	2
2,6-[(CH ₃) ₃ C] ₂	3.58	2
2-CH ₃ -6-(CH ₃) ₃ C	5.52	2
2-(CH ₃) ₂ CH-6-(CH ₃) ₃ C-	5.13	2

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°.

	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

2,4-Dihydroxy-(Uracil)	9.38, 12	39
4,6-Dihydroxy-	5.4	39
2,4,6-Trihydroxy-(Barbituric acid)		

Other (ref. 95)

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

(ref. 96)

2-Methyl- 2-oxazoline	5.5
4-Carbamoyl-2-phenyl- 2-oxazoline	2.9
2-Phenyl- 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

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 ₂ N-	7.25*	4.86*	9.08*	5.37*	5.54*	6.56*	3.90*	2
HO-	-0.36	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 ₂ C	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-Amino-	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-methylquinoxalinium 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
-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 ₂ NCSCSNH ₂)	10.62	77
Ethylenediguanide	1.74, 2.88, 11.34, 11.76	77
Phenyldiguanide	2.16, 10.71	77

Other		
S-Methylisothiurea	9.83	20
N-Phenyl-S-methylisothiurea	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
-Ephedrine	9.22	2
N-Methyl- -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- -Mercaptoethyl-morpholine	6.65, 9.8	
1-Diethylamino-butan- (4)	10.1	5
Methyl-[-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- -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) ₂ SH	12.0	13.96	10.75
X(CH ₂) ₄ SH	12.4	13.25	11.50
X(CH ₂) ₃ SH	13.24	11.14	
X(CH ₂) ₅ SH		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
-Mercaptopropionic acid	10.27	81
Methyl cysteine	6.5 (7.5)	
	81	
p-Cl-thiophenol	7.50	81

Mercaptans, RSH

R		
CH ₃ CCH ₂ -	7.86	32
C ₆ H ₅ CH ₂ -	9.43	82
HOCH ₂ CH(OH)CH ₂ -	9.51	82
CH ₂ =CHCH ₂ -	9.96	82
n-C ₄ H ₉ -	10.66	82
t-C ₅ H ₁₁ -	11.21	82
C ₂ H ₅ OCOCH ₂ -	7.95	82
C ₂ H ₅ OCH ₂ CH ₂ -	9.38	82
HOCH ₂ CH(OH)CH ₂ -	9.66	82
n-C ₃ H ₇ -	a10.65	82
t-C ₄ H 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)

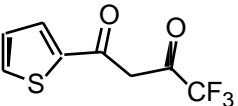
R	R'	R''	pK	pK
CH ₃	CH ₃	(CH ₂) ₅ CH ₃	11.33	12.52
CH ₃	CH ₃	C ₆ H ₅	11.10	12.49
CH ₃	CH ₃	2-ClC ₆ H ₄	11.04	12.73
CH ₃	CH ₃	2-C ₅ H ₄ N	9.80	12.46
CH ₃	CH ₃	2-CH ₃ OC ₆ H ₄	11.47	12.44
CH ₃	CH ₃	3,4-CH ₂ O ₂ C ₆ H ₃	11.39	12.60
CH ₃	CH ₃	3-C ₅ H ₄ N	10.29	12.63
CH ₃	CH ₃	4-CH ₃ OC ₆ H ₄	11.62	12.61
CH ₃	CH ₃	4-(CH ₃) ₂ NC ₆ H ₄	11.50	12.45
CH ₃	CH ₃ OCH ₂	C ₆ H ₅	11.54	12.27
CH ₃	CH ₃ OCH ₂	2-C ₅ H ₄ N	10.95	12.49
CH ₃	CH ₃ OCH ₂	4-(CH ₃) ₂ NC ₆ H ₄	12.13	12.31
CH ₃	CH ₃ OCH ₂	4-CH ₃ OC ₆ H ₄	11.74	12.49
	CH ₃ OCH ₂ COCH ₂ COCH ₃		9.66	
	(CH ₃ CO) ₂ CH(CH ₂) ₃ CH ₃		12.07	

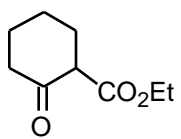
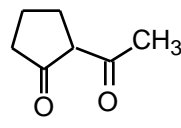
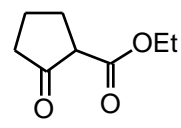
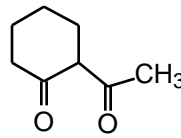
Bis-(β-Diketones) (RCO)-(R'CO)CH-Y-CH(COR)(COR') (in 50% dioxane) (ref. 26)

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) ₂ C ₆ H ₄	11.27	12.15

Bis-(β-Diketones) RCOCH₂CO-Y-COCH₂COR (in 75% dioxane) (ref. 26)

R	Y	pK	pK
C ₆ H ₅	(CH ₂) ₄	12.47	13.09
C ₆ H ₅	(CH ₂) ₅	12.72	13.46
C ₆ H ₅	(CH ₂) ₆	12.60	13.46
C ₆ H ₅	(CH ₂) ₇	13.1 (est.)	
C ₆ H 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 ₃ NO ₂	10.29	74
CH ₃ CHCINO ₂	7	74
CH ₃ COCH ₂ NO ₂	5.1	74
CH(NO ₂) ₃	strong	74
CH ₃ COCHCl ₂	15	74
CH ₃ COCHC ₂ H ₅ CO ₂ C ₂ H ₅	12.7	74
CH ₃ COCHCH ₃ COCH ₃	11	74
CH ₃ COCH ₂ COC ₆ H ₅	9.4	74
C ₆ H ₅ COCH ₂ COCF ₃	6.82	74
CH ₃ COCH ₂ CHO	5.92	74
CH ₃ COCH ₂ CO ₂ CH ₃	10	74
CH ₃ SO ₂ CH ₂ SO ₂ CH ₃	14	74
CH ₃ SO ₂ CH(COCH ₃) ₂	4.3	74
C ₂ H ₅ NO ₂	8.6	74
C ₂ H ₅ O ₂ CCH ₂ NO ₂	5.82	74
CH ₂ (NO ₂) ₂	3.57	74
CH ₃ COCH ₂ Cl	c. 16.5	74
CH ₃ COCH ₂ CO ₂ C ₂ H ₅	10.68	74
CH ₃ COCH ₂ COCH ₃	9	74
CH ₃ COCHBrCOCH ₃	7	74
CH ₃ COCH ₂ COCF ₃	4.7	74
C ₆ H ₅ COCH ₂ NC ₅ H ₅	10.51	74
CH(COCH ₃) ₃	5.85	74
CH ₃ SO ₂ CH ₃	c. 23	74
CH(SO ₂ CH ₃) ₃	strong	74
CH ₂ (CN) ₂	11.81	74
C ₂ H ₅ O ₂ CCH ₂ CN	9	74
CH ₃ CO ₂ C ₂ H ₅	~ 24.5	74
CHC ₂ H ₅ (CO ₂ C ₂ H ₅) ₂	15	74
CH ₃ CONH 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 ₂ C ₂ H ₅) ₂	13.3	74
CH ₃ CO ₂ H	~ 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

References

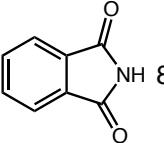
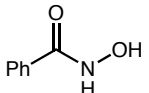
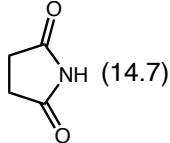
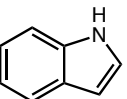
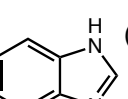
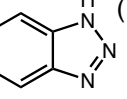
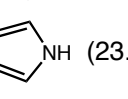
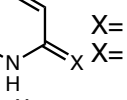
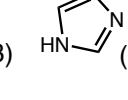
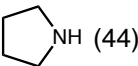
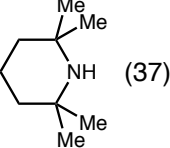
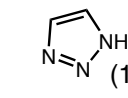
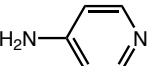
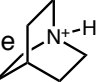
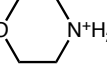
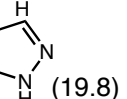
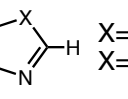
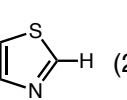
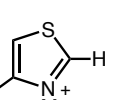
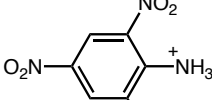
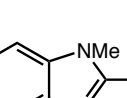
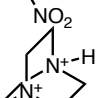
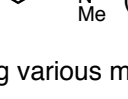
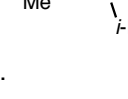
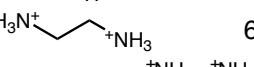


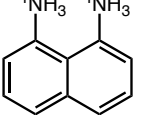
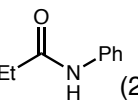
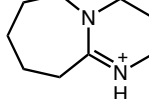
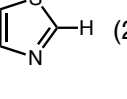
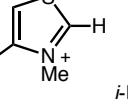
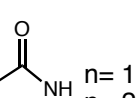
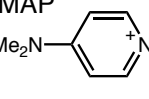
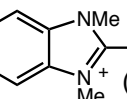
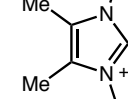
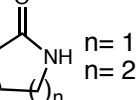
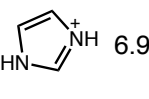
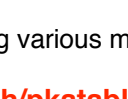

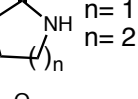


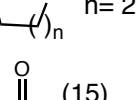
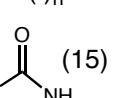
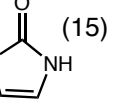
1. Hall, H.K., Jr. *J. Am. Chem. Soc.* **1957**, 79, 5441.
2. Brown, H.C. et al., in Braude, E.A. and F.C. Nachod *Determination of Organic Structures by Physical Methods*, Academic Press, New York, 1955.
3. Hall, H.K., Jr. *J. Am. Chem. Soc.* **1957**, 79, 5439.
4. *Handbook of Chemistry and Physics*, Editor in Chief, Charles D. Hodgman, M.S.; Chemical Rubber Publishing Company, Cleveland, OH, 1951, p. 1636-7.
5. Franzen, V. *Chem. Ber.* **1957**, 90, 623.
6. Dawson, R.M.C. et al., *Data for Biochemical Research*, Oxford, Clarendon Press, 1959.
7. Buist, G.J.; Lucas, H.J. *J. Am. Chem. Soc.* **1957**, 79, 6157.
8. Stevenson, G.W.; Williamson, D. *J. Am. Chem. Soc.* **1958**, 80, 5943.
9. Soloway, S.; Lipschitz, H. *J. Org. Chem.* **1958**, 23, 613.
10. Bissell, E.R.; Finger, M. *J. Org. Chem.* **1959**, 24, 1256.
11. Tuckerman, M.M.; Mayer, J.R.; Nachod, F.C. *J. Am. Chem. Soc.* **1959**, 81, 92.
12. Bissot, T.C.; Parry, R.W.; Campbell, D.H. *J. Am. Chem. Soc.* **1957**, 79, 796.
13. Hinman, R.L. *J. Org. Chem.* **1958**, 23, 1587.
14. Conant, J.B.; Bartlett, P.D. *J. Am. Chem. Soc.* **1932**, 54, 2881.
15. Lindegren, C.R.; Niemann, C. *J. Am. Chem. Soc.* **1949**, 71, 1504.
16. Harnsberger, H.F.; Cochran, E.L.; Szmant, H.H. *J. Am. Chem. Soc.* **1955**, 77, 5048.
17. Pearse, G.A., Jr.; Pflaum, R.T. *J. Am. Chem. Soc.* **1959**, 81, 6505.
18. Bell, R.P.; Higginson, W.C.E. *Proc. Royal Soc.* **1949**, 197, 141.
19. Albert, A.; Goldacre, R.; Phillips, J. *J. Chem. Soc.* **1948**, 2240.
20. Dippy, J.F.J.; Hughes, S.R.C.; Rozanski, A. *J. Chem. Soc.* **1959**, 2492.
21. Edsall, J.T.; Martin, R.B.; Hollingworth, B.R. *PN'As* **1958**, 44, 505.
22. Martin, R.B.; Edsall, J.T.; Wetlaufer, D.B.; Hollingworth, B.R. *JBC* **1958**, 233, 1429.
23. Edsall, J.T.; Wyman and Jeffries, *Biophysical Chemistry*, Academic Press, Inc., New York, 1958.
24. Pearson, R.G.; Dillon, R.L. *J. Am. Chem. Soc.* **1953**, 75, 2439.
25. Ang, K.P. *J. Chem. Soc.* **1959**, 3822.
26. Martin, D.F.; Fernelius, W.C. *J. Am. Chem. Soc.* **1959**, 81, 1509.
27. Ellenbogen, E. *J. Am. Chem. Soc.* **1952**, 74, 5198.
28. Kolthoff, *Treatise on Analytical Chemistry*, New York, Interscience Encyclopedia, Inc., 1959.
29. Edwards, J.O. *J. Am. Chem. Soc.* **1954**, 76, 1540.
30. Bailey, N.A.; Carrington, K.A.; Lott, K.; Symons, M.C.R. *J. Chem. Soc.* **1960**, 290.
31. Brownstein, S.; Stillman, A.E. *J.P.C.* **1959**, 63, 2061.
32. Schwarzenbach *Helv. Chem. Acta.* **1957**, 40, 907.
33. Ingham, J.W.; Morrison, J. *J. Chem. Soc.* **1933**, 1200.
34. Hildebrand, J.H. *Principles of Chemistry*, New York, The Macmillan Company, 1940.
35. Baddiley, in Chargaff, *The Nucleic Acids*, vol. I, New York, Academic Press, 1955.
36. Pabst, OR 1.
37. Bendich, in Chargaff, etc.
38. Jordan, in Chargaff, etc.
39. Albert, A.; Phillips, J.N. *J. Chem. Soc.* **1956**, 1294.
40. Elliott, J.J.; Mason, S.F. *J. Chem. Soc.* **1959**, 2352.
41. Angyal, S.J.; Angyal, C.L. *J. Chem. Soc.* **1952**, 1461.
42. Edward, J.T.; Nielsen, S. *J. Chem. Soc.* **1957**, 5075.
43. Bruice, T.C.; Schmir, G.L. *J. Am. Chem. Soc.* **1958**, 80, 148.
44. Mason, S.F. *J. Chem. Soc.* **1958**, 674.
45. Linnell, R.H. *J. Org. Chem.* **1960**, 25, 290.
46. Jones, R.A.; Katritzky, A.R. *J. Chem. Soc.* **1959**, 1317.
47. Jaffe, H.H.; Doak, G.O. *J. Am. Chem. Soc.* **1955**, 77, 4441.
48. Clarke, K.; Rothwell, K. *J. Chem. Soc.* **1960**, 1885.
49. Keyworth, D.A. *J. Org. Chem.* **1959**, 24, 1355.

50. Gawron, O.; Duggan, M.; Grelechi, C.J. *Anal. Chem.* **1952**, *24*, 969.
51. Sims, P. *J. Chem. Soc.* **1959**, 3648.
52. Fickling, M.M.; Fischer, A.; Mann, B.R.; Packer, J.; Vaughan, J. *J. Am. Chem. Soc.* **1959**, *81*, 4226.
53. Wold, F.; Ballou, C.E. *JBC* **1957**, *227*, 301.
54. McElroy, W.D.; Glass, B. *Phosphorus Metabolism*, Vol. I, Baltimore, Johns Hopkins University Press, 1951.
55. Kumler, W.D.; Eiler, J.J. *J. Am. Chem. Soc.* **1943**, *65*, 2355.
56. VanWazer, J. *Phosphorus and Its Compounds*, Vol. I, New York, Interscience Encyclopedias, Inc., 1958.
57. Freedman, L.D.; Doak, G.O. *Chem. Rev.* **1957**, *57*, 479.
58. Ellman, G.L. *Arch. Biochem. Biophys.* **1958**, *74*, 443.
59. Pascal, I.; Tarbell, D.S. *J. Am. Chem. Soc.* **1957**, *79*, 6015.
60. Bascombe, K.N.; Bell, R.P. *J. Chem. Soc.* **1959**, 1096.
61. Gawron, O.; Draus, F. *J. Am. Chem. Soc.* **1958**, *80*, 5392.
62. Mukherjee, L.M.; Grunwald, E. *JPC* **1958**, *62*, 1311.
63. Ballinger, P.; Long, F.A. *J. Am. Chem. Soc.* **1959**, *81*, 1050.
64. Ballinger, P.; Long, F.A. *J. Am. Chem. Soc.* **1960**, *82*, 795.
65. Haszeldine, R.N. *J. Chem. Soc.* **1953**, 1757.
66. Deno, N.C.; Berkheimer, H.E.; Evans, W.L.; Peterson, H.J. *J. Am. Chem. Soc.* **1959**, *81*, 2344.
67. Gardner, J.N.; Katritzky, A.R. *J. Chem. Soc.* **1957**, 4375.
68. Wise, W.M.; Brandt, W.W. *J. Am. Chem. Soc.* **1955**, *77*, 1058.
69. Fortnum, D.H.; Battaglia, C.J.; Cohen, S.R.; Edwards, J.O. *J. Am. Chem. Soc.* **1960**, *82*, 778.
70. Everett, A.J.; Minkoff, G.J. *TFS* **1953**, *49*, 410.
71. Bauer, L.; Miarka, S.V. *J. Am. Chem. Soc.* **1957**, *79*, 1983.
72. Green, A.L.; Sainsbury, G.L.; Saville, B.; Stansfield, M. *J. Chem. Soc.* **1958**, 1583.
73. Burkhard, R.K.; Sellers, D.E.; DeCou, F.; Lambert, J.L. *J. Org. Chem.* **1959**, *24*, 767.
74. Bell, R.P., *The Proton in Chemistry*, Ithica, Cornell University Press, 1959.
75. Stewart, T.D.; Maeser, S. *J. Am. Chem. Soc.* **1924**, *46*, 2583.
76. Jencks, W.P.; Carriuolo, J. *J. Am. Chem. Soc.* **1960**, *82*, 1778.
77. Bjerrum, J., et al. *Stability Constants*, Chemical Society, London, 1958.
78. Parsons, R. *Handbook of Electrochemical Constants*, London, Butterworths, 1959.
79. Bower, V.E.; Robinson, R.A. *JPC* **1960**, *64*, 1078.
80. Candlin, J.P. *J. Chem. Soc.* **1960**, 4236.
81. Danehy, J.P.; Noel, C.J. *J. Am. Chem. Soc.* **1960**, *82*, 2511.
82. Kreevoy, M.M. et al. *J. Am. Chem. Soc.* **1960**, *82*, 4899.
83. Kabachnik, M.I., et al. *Tetrahedron* **1960**, *9*, 10.
84. Bjerrum, J., et al. *Stability Constants*, Chemical Society, London, 1958.
85. Crutchfield, M.M.; Edwards, J.O. *J. Am. Chem. Soc.* **1960**, *82*, 3533.
86. Lane, T.J.; Quinlan, K.P. *J. Am. Chem. Soc.* **1960**, *2994*, 2997.
87. Moeller, T.; Ferrus, R. *JPC* **1960**, *64*, 1083.
88. Bryson, A. *J. Am. Chem. Soc.* **1960**, *82*, 4558, 4862, 4871.
89. Henderson, W.A., Jr.; Streuli, C.A. *J. Am. Chem. Soc.* **1960**, *82*, 5791.
90. Edwards, J.O. et al. *J. Am. Chem. Soc.* **1960**, *82*, 778.
91. Bell, R.P.; McTigue, P.T. *J. Chem. Soc.* **1960**, 2983.
92. Li, N.C. et al. *J. Am. Chem. Soc.* **1960**, *82*, 3737.
93. Cohen, W.; Erlanger, B.F. *J. Am. Chem. Soc.* **1960**, *82*, 3928.
94. Olson, D.C.; Margerum, D.W. *J. Am. Chem. Soc.* **1960**, *82*, 5602.
95. Ratner, S.; Clarke, H.T. *J. Am. Chem. Soc.* **1937**, *59*, 200.
96. Porter, G.R.; Rydon, H.N.; Schofield, J.A. *Nature* **1958**, *182*, 927.

Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O(DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
INORGANIC ACIDS			CARBOXYLIC ACIDS			ALCOHOLS			PROTONATED SPECIES		
H ₂ O	15.7	(32)				HOH	15.7	(31.2)			-12.4
H ₃ O ⁺	-1.7		X= CH ₃	4.76	(12.3)	MeOH	15.5	(27.9)			-7.8
H ₂ S	7.00		CH ₂ NO ₂	1.68		<i>i</i> -PrOH	16.5	(29.3)			-6.2
HBr	-9.00	(0.9)	CH ₂ F	2.66		<i>t</i> -BuOH	17.0	(29.4)			-6.5
HCl	-8.0	(1.8)	CH ₂ Cl	2.86		<i>c</i> -hex ₃ COH	24.0				-3.8
HF	3.17	(15)	CH ₂ Br	2.86		CF ₃ CH ₂ OH	12.5	(23.5)			-2.05
HOCl	7.5		CH ₂ I	3.12		(CF ₃) ₂ CHOH	9.3	(18.2)			-2.2
HClO ₄	-10		CHCl ₂	1.29		C ₆ H ₅ OH	9.95	(18.0)			-1.8
HCl	-8.0	(1.8)	CCl ₃	0.65		<i>m</i> -O ₂ NC ₆ H ₄ OH	8.4			0.79	(+1.63)
HF	3.17	(15)	CF ₃	-0.25		<i>p</i> -O ₂ NC ₆ H ₄ OH	7.1	(10.8)			(+5.55)
HOCl	7.5		H	3.77		<i>p</i> -OMeC ₆ H ₄ OH	10.2	(19.1)			
HClO ₄	-10		HO	3.6, 10.3		2-naphthol		(17.1)			
HCl	-8.0	(1.8)	C ₆ H ₅	4.2	(11.1)	OXIMES & HYDROXAMIC ACIDS					
HF	3.17	(15)	<i>o</i> -O ₂ NC ₆ H ₄	2.17			11.3	(20.1)			
HOCl	7.5		<i>m</i> -O ₂ NC ₆ H ₄	2.45			8.88	(13.7)			
HClO ₄	-10		<i>p</i> -O ₂ NC ₆ H ₄	3.44				(18.5)			
HCl	-8.0	(1.8)	<i>o</i> -ClC ₆ H ₄	2.94		PEROXIDES					
HF	3.17	(15)	<i>m</i> -ClC ₆ H ₄	3.83		MeOOH	11.5				
HOCl	7.5		<i>p</i> -ClC ₆ H ₄	3.99		CH ₃ CO ₃ H	8.2				
HClO ₄	-10		<i>o</i> -(CH ₃) ₃ N ⁺ C ₆ H ₄	1.37							
HCl	-8.0	(1.8)	<i>p</i> -(CH ₃) ₃ N ⁺ C ₆ H ₄	3.43							
HF	3.17	(15)	<i>p</i> -OMeC ₆ H ₄	4.47							
HOCl	7.5										
HClO ₄	-10		R= H	4.25							
HCl	-8.0	(1.8)	<i>trans</i> -CO ₂ H	3.02, 4.38							
HF	3.17	(15)	<i>cis</i> -CO ₂ H	1.92, 6.23							

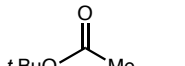
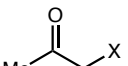
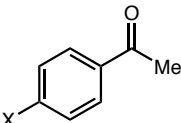
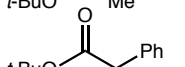
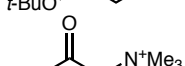
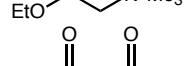

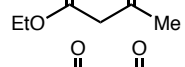
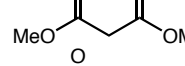
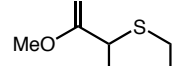
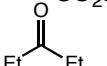

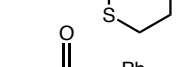
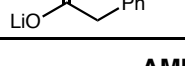
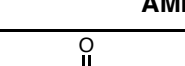
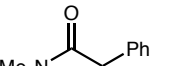
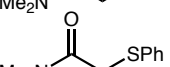
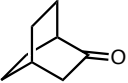
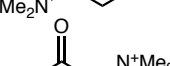
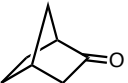
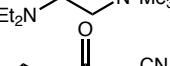
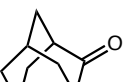
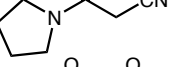

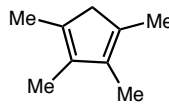
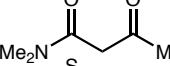
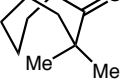
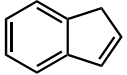
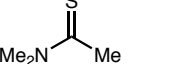

*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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

Substrate	pKa	H ₂ O	(DMSO)	Substrate	pKa	H ₂ O	(DMSO)	Substrate	pKa	H ₂ O	(DMSO)	Substrate	pKa	H ₂ O	(DMSO)
PROTONATED NITROGEN				AMINES				IMIDES				HYDROXAMIC ACID & AMIDINES			
N ⁺ H ₄	9.2	(10.5)		HN ₃	4.7	(7.9)			8.30				8.88	(13.7)	
EtN ⁺ H ₃	10.6			NH ₃	38	(41)			(14.7)			R= Me	(17.3)		
<i>i</i> -Pr ₂ N ⁺ H ₂	11.05			<i>i</i> -Pr ₂ NH	(36 THF))			Ac ₂ NH	(17.9)			R= Ph	(15.0)		
Et ₃ N ⁺ H	10.75	(9.00)		TMS ₂ NH	26(THF)	(30)		SULFONAMIDE				HETEROCYCLES			
PhN ⁺ H ₃	4.6	(3.6)		PhNH ₂	(30.6)			RSO ₂ NH ₂	R = Me	(17.5)			(20.95)		(16.4)
PhN ⁺ (Me) ₂ H	5.20	(2.50)		Ph ₂ NH	(25.0)				Ph	(16.1)			(11.9)		(23.0)
Ph ₂ N ⁺ H ₂	0.78			NCNH ₂	(16.9)			MeSO ₂ NHPh	CF ₃	6.3	(9.7)		X= O (24)		(18.6)
2-naphthal-N ⁺ H ₃	4.16				(44)				Ph	(18.9)		X= S (13.3)			
H ₂ NN ⁺ H ₃	8.12				(37)			PhSO ₂ NHNH ₂		(17.2)		X= O (14.8)		(13.9)	
HON ⁺ H ₃	5.96				(26.5)			PhNHNHPh		(26.1)		X= S (11.8)			
Quinuclidine 	11.0	(9.80)		AMIDES & CARBAMATES				GUANIDINIUM, HYDRAZONES, -IDES, & -INES				PROTONATED HETEROCYCLES			
Morpholine 	8.36			R= H	(23.5)			Me ₂ N=C=NMe ₂	(13.6)				(19.8)		(24.4)
N-Me morpholine	7.38			R= CH ₃	15.1	(25.5)		Ph=C=NMe ₂	(21.6)				X= O (24)		X= S (27.0)
	-9.3			R= Ph	(23.3)			Ph-C(=O)-NHNH ₂	(18.9)				X= S (11.8)		
DABCO 	2.97, 8.82 (2.97, 8.93)			R= CF ₃	(17.2)			PhSO ₂ NHNH ₂	(17.2)				(29.4)		(16.5)
	6.90, 9.95			(urea) NH ₂	(26.9)			PhNHNHPh	(26.1)				(18.4)		(24)
Proton Sponge 	-9.0, 12.0 (-, 7.50)			OEt	(24.8)			PROTONATED HETEROCYCLES							
PhCN ⁺ H	-10				(21.6)			DBU 	(12)	(estimate)			(29.4)		(16.5)
					12	(20.5)		DMAP 	9.2				(18.4)		(24)
					n = 1	(24.1)			6.95				(18.4)		(24)
					n = 2	(26.4)		R= H (PPTS)	5.21	(3.4)			(18.4)		(24)
								<i>t</i> -Bu	4.95	(0.90)					
								Me	6.75	(4.46)					
								Cl, H	0.72						

*Values <0 for H₂O 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>

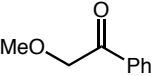
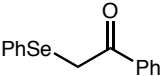
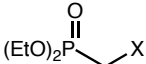
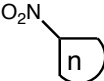
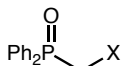
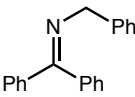
Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
HYDROCARBONS			ESTERS			KETONES					
(Me) ₃ CH	53			24.5	(30.3)						
(Me) ₂ CH ₂	51				(23.6)	X= H		(26.5)	X= H		(24.7)
CH ₂ =CH ₂	50					Ph		(19.8)	OMe		(25.7)
CH ₄	48	(56)			(20.0)	SPh		(18.7)	NMe ₂		(27.5)
	46			11	(14.2)	COCH ₃	9	(13.3)	Br		(23.8)
CH ₂ =CHCH ₃	43	(44)				SO ₂ Ph		(12.5)	CN		(22.0)
PhH	43			13	(15.7)			19-20 (27.1)			
PhCH ₃	41	(43)				<i>i</i> -Pr		(28.3)	n= 4		(25.1)
Ph ₂ CH ₂	33.5	(32.2)			(20.9)	<i>i</i> -Pr		(27.7)	5		(25.8)
Ph ₃ CH	31.5	(30.6)			[30.2 (THF)]	t-Bu		(26.3)	6		(26.4)
HCCH	24		AMIDES			Ph			7		(27.7)
PhCCH	23	(28.8)			(26.6)	X= H		(24.7)	8		(27.4)
XC ₆ H ₄ CH ₃						CH ₃		(24.4)			(28.1)
X= <i>p</i> -CN		(30.8)			(25.9)	Ph		(17.7)			(29.0)
<i>p</i> -NO ₂		(20.4)			(24.9)	COCH ₃		(14.2)			(25.5)
<i>p</i> -COPh		(26.9)			(17.2)	COPh		(13.3)			
		(26.1)			(18.2)	CN		(10.2)			(32.4)
	20	(20.1)			(25.7)	F		(21.6)			
	15	(18.0)				OMe		(22.85)			
H ₂	~36					OPh		(21.1)			
						SPh		(16.9)			
						SePh		(18.6)			
						NPh ₂		(20.3)			
						N ⁺ Me ₃		(14.6)			
						NO ₂		(7.7)			
						SO ₂ Ph		(11.4)			

*Values <0 for H₂O 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 ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)
NITRILES			SULFIDES			SULFOXIDES			SULFONES		
NC-CH ₂ -X			PhSCH ₂ X								
X= H	(31.3)		X= Ph	(30.8)		X= H	(35.1)		X= H	(29.0)	
CH ₃	(32.5)		CN	(20.8)			(29.0)		CH ₃	(31.0)	
Ph	(21.9)		COCH ₃	(18.7)		X= Ph	(29.0)		<i>t</i> -Bu	(31.2)	
COPh	(10.2)		COPh	(16.9)					Ph	(23.4)	
CONR ₂	(17.1)		NO ₂	(11.8)		X= H	(33)		CH=CH ₂	(22.5)	
CO ₂ Et	(13.1)		SPh	(30.8)		Ph	(27.2)		CH=CHPh	(20.2)	
CN	11	(11.1)	SO ₂ Ph	(20.5)		SOPh	(18.2)		CCH	(22.1)	
OPh	(28.1)		SO ₂ CF ₃	(11.0)			(24.5)		CCPh	(17.8)	
N ⁺ Me ₃	(20.6)		POPh ₂	(24.9)		SULFONIUM			COPh	(11.4)	
SPh	(20.8)		MeSCH ₂ SO ₂ Ph	(23.4)		Me ₃ S ⁺ =O	(18.2)		COMe	(12.5)	
SO ₂ Ph	(12.0)		PhSCHPh ₂	(26.7)			(16.3)		OPh	(27.9)	
HETERO-AROMATICS			(PhS) ₃ CH	(22.8)		SULFIMIDES & SULFOXIMINES			N ⁺ Me ₃	(19.4)	
	(28.2)		(PrS) ₃ CH	(31.3)					CN	(12.0)	
	(30.1)			(23.0)					NO ₂	(7.1)	
	(26.7)			(30.5)		R= Me	(27.6)		SMe	(23.5)	
	(25.2)		X= Ph	(30.7)		<i>i</i> -Pr	(30.7)		SPh	(20.5)	
	(30.2)		CO ₂ Me	(20.8)			(24.5)		SO ₂ Ph	(12.2)	
	(30.0)		CN	(19.1)					PPh ₂	(20.2)	
			RSCH ₂ CN				(33)			(22.3)	
			R= Me	(24.3)						(31.1)	
			Et	(24.0)						(18.8)	
			<i>i</i> -Pr	(23.6)			(14.4)			(21.8)	
			<i>t</i> -Bu	(22.9)						(26.6)	
			PhSCH=CHCH ₂ SPh	(26.3)			(20.7)			(32.8)	
			BuSH	10-11	(17.0)				(PhSO ₂) ₂ CH ₂ Me	(14.3)	
			PhSH	≈7	(10.3)						

*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	Substrate	pKa	H ₂ O (DMSO)	REFERENCES
ETHERS			PHOSPHONIUM			NITRO			DMSO: JACS <u>97</u> , 7007 (1975) JACS <u>97</u> , 7160 (1975) JACS <u>97</u> , 442 (1975) JACS <u>105</u> , 6188 (1983) JOC <u>41</u> , 1883 (1976) JOC <u>41</u> , 1885 (1976) JOC <u>41</u> , 2786 (1976) JOC <u>41</u> , 2508 (1976) JOC <u>42</u> , 1817 (1977) JOC <u>42</u> , 321 (1977) JOC <u>42</u> , 326 (1977) JOC <u>43</u> , 3113 (1978) JOC <u>43</u> , 3095 (1978) JOC <u>43</u> , 1764 (1978) JOC <u>45</u> , 3325 (1980) JOC <u>45</u> , 3305 (1980) JOC <u>45</u> , 3884 (1980) JOC <u>46</u> , 4327 (1981) JOC <u>46</u> , 632 (1981) JOC <u>47</u> , 3224 (1982) JOC <u>47</u> , 2504 (1982) Acc. Chem. Res. <u>21</u> , 456 (1988) Unpublished results of F. Bordwell
CH ₃ OPh	(49)		P ⁺ H ₄	-14		RNO ₂			
MeOCH ₂ SO ₂ Ph	(30.7)		MeP ⁺ H ₃	2.7		R= CH ₃	≈10	(17.2)	
PhOCH ₂ SO ₂ Ph	(27.9)		Et ₃ P ⁺ H	9.1		CH ₂ Me		(16.7)	
PhOCH ₂ CN	(28.1)		Ph ₃ P ⁺ CH ₃	(22.4)		CHMe ₂		(16.9)	
	(22.85)		Ph ₃ P ⁺ <i>i</i> -Pr	(21.2)		CH ₂ Ph		(12.2)	
SELENIDES			PHOSPHONATES & PHOSPHINE OXIDES			CH ₂ Bn		(16.2)	
	(18.6)					CH ₂ SPh		(11.8)	
PhSeCHPh ₂	(27.5)		X= Ph	(27.6)		CH ₂ SO ₂ Ph		(7.1)	
(PhSe) ₂ CH ₂	(31.3)		CN	(16.4)		CH ₂ COPh		(7.7)	
PhSeCH ₂ Ph	(31.0)		CO ₂ Et	(18.6)					
PhSeCH=CHCH ₂ SePh	(27.2)		Cl	(26.2)		n= 3		(26.9)	
AMMONIUM			SiMe ₃	(28.8)		4		(17.8)	
Me ₃ N ⁺ CH ₂ X						5		(16.0)	
X= CN	(20.6)		X= SPh	(24.9)		6		(17.9)	
SO ₂ Ph	(19.4)		CN	(16.9)		7		(15.8)	
COPh	(14.6)		PHOSPHINES			IMINES			Water: Advanced Org. Chem., 3rd Ed. J. March (1985) Unpublished results of W. P. Jencks
CO ₂ Et	(20.0)		Ph ₂ PCH ₂ PPh ₂	(29.9)				(24.3)	
CONEt ₂	(24.9)		Ph ₂ PCH ₂ SO ₂ Ph	(20.2)		Oxime ethers are ~ 10 pka units less acidic than their ketone counterparts Streitwieser, JOC 1991, 56, 1989			THF: JACS <u>110</u> , 5705 (1988)

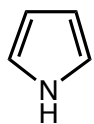
*Values <0 for H₂O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

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

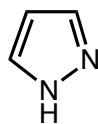
DMSO Acidities of Common Heterocycles

Bordwell, ACR, 1988, 21, 456

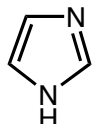
Bordwell <http://www.chem.wisc.edu/areas/reich/pkatable/index.htm>



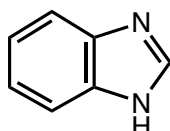
23.0



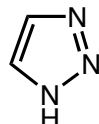
19.8



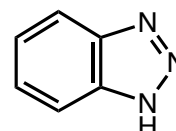
18.6



16.4



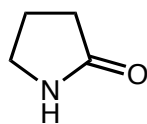
13.9



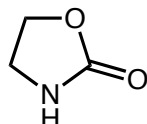
11.9



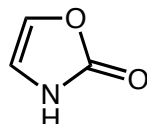
18.0



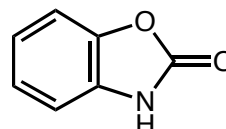
24.0



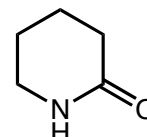
20.8



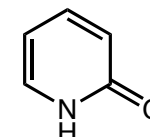
15.0



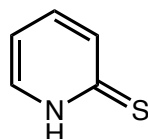
12.1



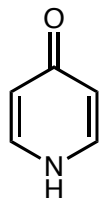
26.4



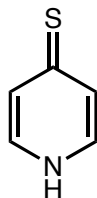
24.0



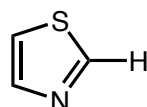
13.3



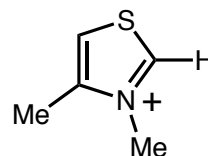
14.8



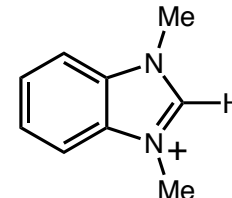
11.8



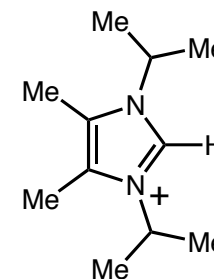
29.4



16.5



18.4



24