

**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

*pKa Data Compiled by R. Williams***ACIDS**

Compound	pK	Ref.			
			H <sub>3</sub> PO <sub>2</sub>	2.0, 2.23*	28
			H <sub>2</sub> PO <sub>4</sub> <sup>-</sup>	7.21*	77
AgOH	3.96	4	HPO <sub>4</sub> <sup>-</sup>	12.32*	77
Al(OH) <sub>3</sub>	11.2	28	H <sub>3</sub> PO <sub>3</sub>	2.0	28
As(OH) <sub>3</sub>	9.22	28	H <sub>2</sub> PO <sub>3</sub> <sup>-</sup>	6.58*	77
H <sub>3</sub> AsO <sub>4</sub>	2.22, 7.0, 13.0	28	H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	1.52*	77
H <sub>2</sub> AsO <sub>4</sub> <sup>-</sup>	6.98*	77	H <sub>3</sub> P <sub>2</sub> O <sub>7</sub> <sup>-</sup>	2.36*	77
HAsO <sub>4</sub> <sup>*</sup>	11.53*	77	H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> <sup>=</sup>	6.60*	77
As <sub>2</sub> O <sub>3</sub>	0	4	HP <sub>2</sub> O <sub>7</sub> <sup>=</sup>	9.25*	77
H <sub>3</sub> AsO <sub>3</sub>	9.22*		HReO <sub>4</sub>	-1.25	30
H <sub>3</sub> BO <sub>3</sub>	9.23*	28	HSCN	4.00	34
H <sub>2</sub> B <sub>4</sub> O <sub>7</sub>	4.00	34	H <sub>2</sub> SeO <sub>3</sub>	2.6, 8.3, 2.62*	28
HB <sub>4</sub> O <sub>7</sub>	9.00	34	HSeO <sub>3</sub>	8.32	77
Be(OH) <sub>2</sub>	3.7	4	H <sub>2</sub> SeO <sub>4</sub>	Strong, 2.0	28
HBr	-9.00	31	HSeO <sub>4</sub>	2.00	34
HOBr	8.7	28	H <sub>3</sub> SiO <sub>3</sub>	10.0	34
HOCl	7.53, 7.46	28, 33	H <sub>2</sub> SO <sub>3</sub>	1.9, 7.0, 1.76*	28, 77
HClO <sub>2</sub>	2.0	28	H <sub>2</sub> SO <sub>4</sub>	-3.0, 1.9	28
HClO <sub>3</sub>	-1.00	28	HSO <sub>3</sub>	7.21*	77
HClO <sub>4</sub> (70%)	-10.00	31	HSO <sub>4</sub> <sup>-</sup>	1.99*	77
CH <sub>3</sub> SO <sub>3</sub> H	-0.6	31	H <sub>2</sub> S <sub>2</sub> O <sub>4</sub>	1.9	29
HCN	9.40	34	H <sub>2</sub> Se	3.89*	77
H <sub>2</sub> CO <sub>3</sub>	6.37, 6.35*, 3.58	34, 32	HSe <sup>-</sup>	11.00*	77
HCO <sub>3</sub>	10.33*		H <sub>2</sub> S	7.00*	77
H <sub>2</sub> CrO <sub>4</sub>	-0.98	30	HS <sup>-</sup>	12.92*	77
HCrO <sub>4</sub>	6.50*	2, 30	HSbO <sub>2</sub>	11.0	34
HOCN	3.92	34	HTe	5.00	34
HZ	3.17*, 0.59*	77	H <sub>2</sub> Te	2.64, 11.0	34, 78
H <sub>2</sub> GeO <sub>3</sub>	8.59, 12.72	34, 78	H <sub>2</sub> TeO <sub>3</sub>	2.7, 8.0	28
Ge(OH) <sub>4</sub>	8.68, 12.7	28	Te(OH) <sub>6</sub>	6.2, 8.8	28
HI	-10.0	31	H <sub>2</sub> VO <sub>4</sub> <sup>-</sup>	8.95	30
HOI	11.0	28	HVO <sub>4</sub> <sup>=</sup>	14.4	30
HIO <sub>3</sub>	0.8	28	H <sub>2</sub> CrO <sub>4</sub>	0.74	77
H <sub>4</sub> IO <sub>6</sub> <sup>-</sup>	6.00	34	HOCN	3.73	77
H <sub>5</sub> IO <sub>6</sub>	1.64, 1.55, 8.27	34, 28	HSCN	0.85	77
HMnO <sub>4</sub>	-2.25	30	H <sub>3</sub> PO <sub>2</sub>	1.07	77
NH <sub>3</sub> OH <sup>*</sup>	5.98*		H <sub>3</sub> PO <sub>4</sub>	2.12*	77
NH <sub>4</sub> <sup>*</sup>	9.24*	77	H <sub>2</sub> S <sub>2</sub> O <sub>3</sub>	0.60*, 1.72*	77
HN <sub>3</sub>	4.72*	77	H <sub>3</sub> AuO <sub>3</sub>	13.3, 16.0	78
HNO <sub>2</sub>	3.29	28	H <sub>3</sub> GaO <sub>3</sub>	10.32, 11.7	78
HNO <sub>3</sub>	-1.3	28	H <sub>5</sub> IO <sub>6</sub>	3.29, 6.70, 15.0	78
N <sub>2</sub> H <sub>5</sub> <sup>+</sup>	7.99*	77		(see above!)	
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	7.05	34	H <sub>4</sub> V <sub>6</sub> O <sub>17</sub>	1.96	78
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> <sup>-</sup>	11.0	34	H <sub>2</sub> NSO <sub>3</sub> H	1.0	80
H <sub>2</sub> OsO <sub>5</sub>	12.1	34			
H <sub>2</sub> O	15.7	none			
H <sub>3</sub> O <sup>+</sup>	-1.7	none			
Pb(OH) <sub>2</sub>	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 <sub>2</sub> O <sub>3</sub> P(CH <sub>2</sub> ) <sub>4</sub> PO <sub>3</sub> H <sub>2</sub>	<2, 2.75, 7.54, 8.38	57
H <sub>2</sub> O <sub>3</sub> P(CH <sub>2</sub> ) <sub>3</sub> PO <sub>3</sub> H <sub>2</sub>	<2, 2.65, 7.34, 8.35	57
H <sub>2</sub> O <sub>3</sub> PCH <sub>2</sub> CH(CH <sub>3</sub> )PO <sub>3</sub> H <sub>2</sub>	<2, 2.6, 7.00, 9.27	57
H <sub>2</sub> O <sub>3</sub> PCH <sub>2</sub> PO <sub>3</sub> H <sub>2</sub>	<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 <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> CH(COOH)-	1, --	57

CF <sub>3</sub> -	1.16, 3.93	57
CCl <sub>3</sub> -	1.63, 4.81	57
NH <sub>3</sub> <sup>+</sup> CH <sub>2</sub> -	2.35, 5.9	57
(-OOCCH <sub>2</sub> ) <sub>2</sub> NH <sup>+</sup> CH <sub>2</sub> <sup>-</sup>	--, 5.57	57
CHCl <sub>2</sub> -	1.14, 5.61	57
CH <sub>2</sub> Cl-	1.40, 6.30	57
CH <sub>2</sub> Br-	1.14, 6.52	57
(-OOCCH <sub>2</sub> ) <sub>2</sub> NH <sup>+</sup> (CH <sub>2</sub> ) <sub>2</sub> -	--, 6.54	57
CH <sub>2</sub> I-	1.30, 6.72	57
NH <sub>3</sub> <sup>+</sup> CH <sub>2</sub> CH <sub>2</sub> -	2.45, 7.00	57
C <sub>6</sub> H <sub>5</sub> CH=CH-	2.00, 7.1	57
HOCH <sub>2</sub> -	1.91, 7.15	57
C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> <sup>+</sup> (CH <sub>2</sub> ) <sub>3</sub> <sup>-</sup>	2.1, --	57
C <sub>6</sub> H <sub>5</sub> NH(CH <sub>2</sub> ) <sub>3</sub> <sup>-</sup>	--, 7.17	57
Br(CH <sub>2</sub> ) <sub>2</sub> -	2.25, 7.3	57
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> CH(COO <sup>-</sup> )-	--, 7.5	57
C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> -	2.3, 7.55	57
NH <sub>3</sub> <sup>+</sup> (CH <sub>2</sub> ) <sub>4</sub> -	2.55, 7.55	57
NH <sub>3</sub> <sup>+</sup> (CH <sub>2</sub> ) <sub>5</sub> -	2.6, 7.6	57
NH <sub>3</sub> <sup>+</sup> (CH <sub>2</sub> ) <sub>10</sub> -	--, 8.00	57
-OOC(CH <sub>2</sub> ) <sub>10</sub> -	--, 8.25	57
(CH <sub>3</sub> ) <sub>3</sub> SiCH <sub>2</sub> -	3.22, 8.70	57
C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> -	3.3, 8.4	57
(C <sub>6</sub> H <sub>5</sub> )SC-	3.85, 9.00	57

**Arylphosphonic acids**

2X-RC <sub>6</sub> H <sub>3</sub> PO <sub>3</sub> H <sub>2</sub>			
X	R		
Cl	4-O <sub>2</sub> N	1.12, 6.14	57
Br	5-O <sub>2</sub> 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 <sub>3</sub>	1.81, 7.15	57
Cl	4-NH <sub>2</sub>	--, 7.33	57
CH <sub>3</sub> O	4-O <sub>2</sub> N	1.53, 6.96	57
CH <sub>3</sub> O	H	2.16, 7.77	57
CH <sub>3</sub> O	4-O <sub>2</sub> N	--, 8.22	57
HO	4-O <sub>2</sub> N	1.22, 5.39	57
O <sub>2</sub> N	H	1.45, 6.74	57
F	H	1.64, 6.80	57
I	H	1.74, 7.06	57
NH <sub>2</sub> H	--, 7.29	57	
CH <sub>3</sub> H	2.10, 7.68	57	
C <sub>6</sub> H <sub>5</sub>	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	
<b>Phosphonates (Ref. 2)</b>				
<b>X</b>	<b>-H</b>	<b>-H</b>	<b>-NH<sub>3</sub><sup>+</sup></b>	<b>-NH<sub>3</sub><sup>+</sup></b>
X(CH <sub>2</sub> )PO <sub>3</sub> H <sub>2</sub>	2.35	7.1	1.85	5.35
X(CH <sub>2</sub> ) <sub>2</sub> PO <sub>3</sub> H <sub>2</sub>	2.45	7.85	2.45	7.00
X(CH <sub>2</sub> ) <sub>4</sub> PO <sub>3</sub> H <sub>2</sub>			2.55	7.55
X(CH <sub>2</sub> ) <sub>5</sub> PO <sub>3</sub> H <sub>2</sub>			2.6	7.65
X(CH <sub>2</sub> ) <sub>6</sub> PO <sub>2</sub> H <sub>2</sub>	2.6	7.9		
X(CH <sub>2</sub> ) <sub>10</sub> PO <sub>2</sub> H <sub>2</sub>				8.00
Phosphines in acetonitrile, see ref. 89.				

## CARBOXYLIC ACIDS

### Aliphatic

<b>Compound</b>	<b>pK</b>	<b>Ref.</b>
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

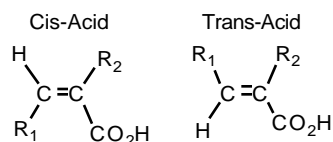
### Acetic acids, substituted

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

\* Indicates thermodynamic values.

**Unsaturated acids (25°)**

Compound	pK	ref.	Compound	pK	ref.
trans-CH <sub>3</sub> -CH=CHCO <sub>2</sub> H	4.69*	20	H-CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.88*	2
cis-CH <sub>3</sub> -CH=CHCO <sub>2</sub> H	4.44*	2	H-CH=CHCO <sub>2</sub> H	4.25*	2
C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.66*	2	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.66*	2
trans-C <sub>6</sub> H <sub>5</sub> -CH=CHCO <sub>2</sub> H	4.44*	2	C <sub>6</sub> H <sub>5</sub> CH=CHCO <sub>2</sub> H**	4.44*	2
m-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.65*		C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.66*	2
	2		C <sub>6</sub> H <sub>5</sub> CH=CHCO <sub>2</sub> H**	4.44	2
m-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CH=CHCO <sub>2</sub> H	4.38*	2	m-ClC <sub>6</sub> H <sub>4</sub> CH=CHCO <sub>2</sub> H**	4.29*	2
m-ClC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H	4.58*	2			

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

R <sub>1</sub>	R <sub>2</sub>	cis-acid	trans-acid	Ref.
H-	H-	4.25*	4.25*	2
CH <sub>3</sub> -	H-	4.44*	4.69*	2
Cl-	H-	3.32	3.65	2
C <sub>6</sub> H <sub>5</sub> -	H-	3.88*	4.44*	2
ClC <sub>6</sub> H <sub>4</sub>	H-	3.91	4.41	2
6-BrC <sub>6</sub> H <sub>4</sub>	H-	4.02	4.41	2
CH <sub>3</sub> -	CH <sub>3</sub> -	4.30	5.02	2
C <sub>6</sub> H <sub>5</sub> -	H-	5.26***	5.58***	2
2,4,6-(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> -	H-	6.12***	5.70***	2
C <sub>6</sub> H <sub>5</sub> -	CH <sub>3</sub> -	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**

<b>Compound</b>	<b>pK</b>	<b>Ref</b>	<b>Compound</b>	<b>pK</b>	<b>Ref</b>
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 <sub>2</sub> H <sub>5</sub> O <sub>2</sub> C-	6.31	2	Br-	6.08	2
NC-	5.90	2	<b>Lysergic acid, etc.</b>		
			ergometrine	6.8, --	2
			Dihydroergometrine	7.4, --	2
			-dihydrolysergol	8.2, --	2

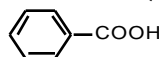
Lysergic acid	7.8, 3.3	2
-dihydrolysergic	8.3, 3.6	2
ergometrinine	7.3, --	2
-dihydrolysergol	8.3, --	2
6-methylergoline	8.85, --	2
isolysergic acid	8.4, 3.4	2
-dihydrolysergic	8.6, 3.6	2

**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 <sub>3</sub> 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 <sub>2</sub> N-	2.17*	3.45*	3.44
CH <sub>3</sub> CO-			
CH <sub>3</sub> SO <sub>2</sub> -		3.64*	3.52*
CH <sub>3</sub> S-			
HS-			
Br-	2.85*	3.81*	4.00*
F-	3.27*	3.87*	4.14*
CH <sub>3</sub> O-	4.09*	4.09*	4.47*
n-C <sub>3</sub> H <sub>7</sub> O-	4.24*	4.20*	4.46*
n-C <sub>4</sub> H <sub>9</sub> O-		4.25*	4.53*

**Benzene Polycarboxylic acids Ref. 2**

Acid	Position of carboxyl	pK <sup>I</sup>	pK <sup>II</sup>	pK <sup>III</sup>	pK <sup>IV</sup>	pK <sup>V</sup>	pK <sup>VI</sup>
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 <sub>6</sub> H <sub>5</sub> O-	3.53*	3.95*	4.52*
CH <sub>3</sub> -	3.91*	4.24*	4.34*
(CH <sub>3</sub> ) <sub>2</sub> CH-			4.35*
(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> -	1.37	3.45	3.43
NC-		3.60*	3.55*
HO <sub>2</sub> C*	2.95*	3.54	3.51
F <sub>3</sub> C-		3.79	
HO-	2.98*	4.08*	4.58*
I-	2.85*	3.86*	
Cl-	2.94*	3.83*	3.99*
(CH <sub>3</sub> ) <sub>3</sub> Si-		4.24*	4.27*
C <sub>2</sub> H <sub>5</sub> O-	4.21*	4.17*	4.45*
i-C <sub>3</sub> H <sub>7</sub> O-	4.24*	4.15*	4.68*
n-C <sub>5</sub> H <sub>11</sub> O-			4.55*
C <sub>6</sub> H <sub>5</sub> -	3.46*		
CH <sub>3</sub> CH <sub>2</sub> -	3.77		4.35*
(CH <sub>3</sub> ) <sub>3</sub> C-	3.46	4.28	4.40*
-HO <sub>3</sub> P-	3.78	4.03	3.95
-O <sub>3</sub> S-		4.15	4.11
H <sub>2</sub> N-	4.98	4.79	4.92
(CH <sub>3</sub> ) <sub>2</sub> N-	8.42	5.10	5.03
-HO <sub>3</sub> As-			4.22
-O <sub>2</sub> C-	5.41**	4.60	4.82
CH <sub>3</sub> 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 <sub>3</sub> -	3.91**	2
2-t-C <sub>4</sub> H <sub>9</sub> -	3.46	2
2,6-(CH <sub>3</sub> ) <sub>2</sub> -	3.21	2
2,3,4,6-(CH <sub>3</sub> ) <sub>4</sub> -	4.00	2
2,3,5,6-(CH <sub>3</sub> ) <sub>4</sub> -	3.52	2
2-C <sub>2</sub> H <sub>5</sub> -	3.77	2
2-C <sub>6</sub> H <sub>5</sub> -	3.46**	2
2,4,6-(CH <sub>3</sub> ) <sub>3</sub> -	3.43	2
2,3,4,5-(CH <sub>3</sub> ) <sub>4</sub> -	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*	
<i>*ionic strength 0.03</i>		2-Methoxyethyliminodiacetic					2.2, 8.96
<i>**thermodynamic</i>		2-Methylthioethyliminodiacetic					2.1, 8.91
		oxalic acid*					1.25, 4.14
		N-n-propylaminoacetic					2.25, 10.03
		N-2-sulfoethyliminodiacetic					1.92, 2.28, 8.16
		-Bromobutyric acid					2.97
		N-(carbamoylmethyl)-imino-diacetic acid					2.30, 6.60
		Cyanomethyliminodiacetic					3.06, 4.34
		, -diaminopropionic acid					1.23, 6.69
		Diethylaminoacetic					2.04, 10.47
		Dimethylaminoacetic					2.08, 9.80
		N-ethylaminoacetic					2.30, 10.10
		Gluconic*					3.86
		-hydroxybutyric					4.39
		-hydroxypropionic					3.73
		Iminodiacetic*					2.98, 9.89
		-iodopropionic*					4.04
		N-isopropylaminoacetic					2.36, 10.06
		-mercaptoputyric					3.53
		N-methylaminoacetic					2.24, 10.01
		Nitrilotriacetic					3.03, 3.07, 10.
		2-Phosphonoethyliminodiacetic					1.95, 2.45, 6.54, 10.46
<b>Carboxylic Acids</b>	<b>Ref. 77</b>						
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						

\*Thermodynamic



## PHENOLS

Compound	pK			Ref.	Compound	pK			Ref.		
Chromotropic acid	5.36, 15.6			6	Resorcinol	--, 9.15 (30°)			50		
o-Methoxyphenol	--, 9.93			50	p-Methoxyphenol	--, 10.16			50		
o-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 <sub>2</sub> N-	7.23*			8.35*	7.14*
(CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> -	7.42			8	8	OCH-	6.79			8.00	7.66
CH <sub>3</sub> SO <sub>2</sub> -				9.33	7.83	NC-				8.61**	7.95
CH <sub>3</sub> CO-				9.19	8.05	CH <sub>3</sub> O <sub>2</sub> C-					8.47*
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> C-					8.50*	n-C <sub>4</sub> H <sub>9</sub> O <sub>2</sub> C-					8.47*
C <sub>3</sub> H <sub>5</sub> CH <sub>2</sub> O <sub>2</sub> 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 <sub>3</sub> S-				9.53	9.53
HO-	9.48			9.44	9.96	HOCH <sub>2</sub> -	9.92*			9.83*	9.82*
CH <sub>3</sub> -	10.28*			10.08	10.19*	C <sub>2</sub> H <sub>5</sub> -	10.2			9.9	10.0
CH <sub>3</sub> O-	9.93			9.65	10.20	H <sub>2</sub> N-	9.71			9.87	10.30
-O <sub>2</sub> C-				9.94*	9.39*	-O <sub>3</sub> S-				9.29	9.03
--O <sub>3</sub> P-				10.2	9.9	--O <sub>3</sub> As					8.37
C <sub>6</sub> H <sub>5</sub> -	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 <sub>3</sub> F <sub>7</sub> •CH(C <sub>2</sub> F <sub>5</sub> )•OH	10.48	65
Chloral hydrate	9.66, 11.0	61	(C <sub>3</sub> F <sub>7</sub> ) <sub>2</sub> CH•OH	10.52	65
Trifluoroethanol	11.4, 12.43	63	62 Carbonium ions		
CF <sub>3</sub> CH <sub>2</sub> OH	11.8	63	<b>Triphenylmethanols in</b>		
CF <sub>3</sub> CH(OH)CH <sub>3</sub>	12.43	10	4,4,4-Trimethoxy	H <sub>2</sub> SO <sub>4</sub> .82, HClO <sub>4</sub> .82, HNO <sub>3</sub> .82	ref .80 66
CF <sub>3</sub> CH <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> OH	11.4**	63	4,4'-Dimethoxy	-1.24	-1.14 -1.11 66
C <sub>3</sub> F <sub>7</sub> CH <sub>2</sub> OH	10.6**	63	4-Methoxy	-3.40	-3.59 -3.41 66
(C <sub>3</sub> F <sub>7</sub> ) <sub>2</sub> CHOH	13.55	64	4-Methyl	-5.41	-5.67 66
HCCCH <sub>2</sub> OH	14.1	64	4-Trideuteriomethyl-	5.43	5.67 66
C(CH <sub>2</sub> OH) <sub>4</sub>	4.4	64	3,3',3''-Trimethyl-	6.35	-5.95 66
HOCH <sub>2</sub> CHOHCH <sub>2</sub> OH	14.77	64	<b>Unsubstituted triphenyl-</b>		
HOCH <sub>2</sub> CH <sub>2</sub> OH	14.82	64	methanol-	6.63	-6.89 6.60 66
CH <sub>3</sub> CCH <sub>2</sub> OH	15.54		64 4,4,4;-Trichloro-		7.74- 8.01 66
CH <sub>3</sub> OH	15.52		64 4-Nitro-		9.15- 9.76 66
CH <sub>2</sub> =CHCH <sub>2</sub> OH	15.74	64	CCl <sub>3</sub> CH <sub>2</sub> OH	11.8***	
H <sub>2</sub> O	16	64	CF <sub>3</sub> CH <sub>2</sub> OH	11.3***	
CH <sub>3</sub> CH <sub>2</sub> OH					
<b>Substituent effects for ionization of RCH<sub>2</sub>OH</b>					
<b>R</b>					
CCl-3	12.24,11.80	64,65	<b>Hydroxamic acids</b>		
CF <sub>3</sub> -	12.37	64	Furo-	8.45	72
CHF <sub>2</sub> CH <sub>2</sub> -	12.74	64	Glycine	7.40	72
CHCl <sub>2</sub> -	12.89	64	Hippuro-	8.80	72
CHEC-	13.55	64	isoNicotin	7.85	72
H <sub>2</sub> Cl-	14.31	64	64 p-Methylbenz-		8.90 72
CH <sub>3</sub> CCH <sub>2</sub> -	14.8	64	Nicotin-		8.30 72
HOCH <sub>2</sub>	15.1		Nicotin-methiodide	6.46	72
H-	15.5	64	m-Nitrobenz-	8.07	72
CH <sub>2</sub> =CH-	15.5	64	Picolin	8.50	72
CH <sub>3</sub> -(extrap)	(15.9)	64	Pyrimidine-2-carbox-	7.88	72
CF <sub>3</sub> C(CH <sub>3</sub> ) <sub>2</sub> OH	11.6	64	Salicyl-	7.43	72
HOCH <sub>2</sub> CF <sub>2</sub> CH <sub>2</sub> OH	11	64	Tropo-		9.09 72
Primary alcohols=R•CH <sub>2</sub> •OH and					
Secondary alcohols in 50% alcohol					
C <sub>2</sub> F <sub>5</sub>	11.35	65	<b>Other oxygen acids</b>		
C <sub>4</sub> F <sub>9</sub>	11.35	65	Trimethylamine-n-oxide	4.6	18
C <sub>5</sub> F <sub>11</sub>	11.37	65	Dimethylglyoxime		12.84 77
C <sub>7</sub> F <sub>15</sub>	11.35	65	(50% dioxane)		
CHF <sub>2</sub>	12.00	65	O-methyl ether	12.92	77
CF <sub>2</sub> Cl	11.63	65	Tropolone	12a	77
CHF <sub>2</sub> CF <sub>2</sub>	11.34	65	-Bromotropolone	6.95 <sup>a</sup>	77
CHF <sub>2</sub> •(CF <sub>2</sub> ) <sub>2</sub>	11.35	65	Acetald hydrate	13.48	91
CF <sub>3</sub> •CH <sub>2</sub>	12.7	65	Formald hydrate	13.29	91
CF <sub>3</sub> •(CH <sub>2</sub> ) <sub>2</sub>	12.9	65			
CF <sub>3</sub> •CHMe•OH	11.28	65			
C <sub>3</sub> F <sub>7</sub> •CHMe•OH	11.38	65			
C <sub>3</sub> F <sub>7</sub> CH <sub>2</sub> Et•OH	11.37	65			
C <sub>3</sub> F <sub>7</sub> CH <sub>2</sub> Pr•OH	11.37	65			
C <sub>3</sub> F <sub>7</sub> •CH(CF <sub>3</sub> )•OH	10.46	65			

<sup>a</sup>50% dioxane

\*\*\*50 aqueous ethanol

## OTHER OXYGEN ACIDS

Compound	pK	Ref.
<b>Pyridine oxides</b>		
4-Aminopyridine 1-oxide	3.69	67
4-Dimethylaminopyridine 1-oxide	3.88	67
4-Dimethylaminopyridine 1-oxide	3.88	67
4-Dimethylamino-1-methoxypyridinium perchlorate	>11	67
2-Methylaminopyridine 1-oxide	2.61	67
2-Amino-1-methoxypyridinium perchlorate	12.4	67
4-Hydroxypyridine 1-oxide	2.45	67
4-Methoxypyridine 1-oxide	2.05	67
1-Methoxypyridi-4-one	2.57	67
2-Hydroxypyridine 1-oxide	-0.8	67
2-Ethoxypyridine 1-oxide	1.18	67
1-Methoxypyrid-2-one	-1.3	
4-Methylaminopyridine 1-oxide	3.85	67
4-Amino-1-methoxypyridinium perchlorate	>11	67
2-Aminopyridine 1-oxide	2.67	67
2-Dimethylaminopyridine 1-oxide	2.27	67
2-Methylamino-1-methoxypyridinium toluene-p-sulphonate	>11	67
4-Benzyloxypyridine 1-oxide	1.99	67
1-Benzyloxypyrid-4-one	2.58	67
2-Methoxypyridine 1-oxide	1.23	67
1-Benzyloxypyrid-2-one	-1.7	67
<b>Pyridine 1-oxides</b>		
<b>R</b>	<b>pK</b>	<b>Ref.</b>
4-CH <sub>3</sub>	1.29	47
3-CH <sub>3</sub>	1.08	47
3,4-(CH) <sub>4</sub>	1.01	47
3-COOC <sub>4</sub> H <sub>9</sub>	0.03	47
4-NO <sub>2</sub>	-1.7	47
3-NH <sub>2</sub>	1.47	47
H	0.79	47
3-COOH	0.09	47
4-COOH	-0.48	47

## Peroxides ROOH (Ref. 70)

H	CH <sub>3</sub>	C <sub>2</sub> H <sub>5</sub>	iso-C <sub>3</sub> H <sub>7</sub>	tert-C <sub>4</sub> H <sub>9</sub>	iso-C <sub>4</sub> H <sub>9</sub>
11.6	11.5	11.8	12.1	12.8	12.8

<b>Oximes</b>	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

<b>sulfinic acids</b>		
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

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

**Amino Acids**

Compound	pK -COOH	Ref. -NH <sub>3</sub>
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
<b>Peptides</b>		
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	$\alpha$ -NH <sub>2</sub>	$\epsilon$ -NH <sub>2</sub>	$\epsilon$ -NH <sub>2</sub>	$\epsilon$ -NH <sub>2</sub>	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			
<b>NITROGEN COMPOUNDS</b>							
<b>Aliphatic Amines</b>							
	<b>pK</b>	<b>ref.</b>					
Ammonia	9.21	1		n-Propyl-	10.53	1	
Primary Amines				Trimethylsilylmethyl-	10.96	1	
-Alanine ester	9.13	1		CH <sub>3</sub> ONH <sub>2</sub>	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*	?	
<b>X</b>	<b>XNH<sub>3</sub><sup>+</sup></b>	<b>XCH<sub>2</sub>NH<sub>3</sub><sup>+</sup></b>	<b>X(CH<sub>2</sub>)<sub>2</sub>NH<sub>3</sub><sup>+</sup></b>	<b>X(CH<sub>2</sub>)<sub>3</sub>NH<sub>3</sub><sup>+</sup></b>	<b>X(CH<sub>2</sub>)<sub>4</sub>NH<sub>3</sub><sup>+</sup></b>	<b>X(CH<sub>2</sub>)<sub>5</sub>NH<sub>3</sub><sup>+</sup></b>	<b>ref.</b>
H-	9.25*	10.64*	10.67*	10.58*	10.61*	10.63*	2
HF <sub>2</sub> C-		7.52					
RO <sub>2</sub> C-		7.75	9.13	9.71	10.15*	10.37	2
HO-	5.96*		9.50*				
C <sub>6</sub> H <sub>5</sub> -	4.58*	9.37*	9.83*	10.20*	10.39*	10.49*	2
H <sub>2</sub> N-	8.12*		9.98*	10.65*	10.84*	11.05*	2
H <sub>2</sub> C=CH-		9.69					
CH <sub>3</sub> -	10.64*	10.67*	10.58*	10.61*	10.63*	10.64*	2
<b>X</b>	<b>-H</b>	<b>-NH<sub>3</sub><sup>+</sup></b>	<b>-CO<sub>2</sub><sup>-</sup></b>	<b>-SO<sub>3</sub><sup>-</sup></b>	<b>-PO<sub>3</sub><sup>-</sup></b>		<b>2</b>
X-NH <sub>3</sub> <sup>+</sup>	9.25*	-.88		1	10.25		
X(CH <sub>2</sub> ) <sub>2</sub> NH <sub>3</sub> <sup>+</sup>	10.64			9.77	5.75	10.8	
X(CH <sub>2</sub> ) <sub>2</sub> NH <sub>3</sub> <sup>+</sup>	10.67			10.19	9.20	10.8	
X(CH <sub>2</sub> ) <sub>4</sub> NH <sub>3</sub> <sup>+</sup>	10.61	9.31		10.77	10.65	10.9	
X(CH <sub>2</sub> ) <sub>5</sub> NH <sub>3</sub> <sup>+</sup>	10.63	9.74		10.75	10.95	11.0	
X(CH <sub>2</sub> ) <sub>8</sub> NH <sub>3</sub> <sup>+</sup>	10.65	10.10					
X(CH <sub>2</sub> ) <sub>10</sub> NH <sub>3</sub> <sup>+</sup>	10.64				11.35	11.25	
X(CH <sub>2</sub> ) <sub>3</sub> NH <sub>3</sub> <sup>+</sup>	10.58	8.59		10.43	10.05		
<b>Secondary amines</b>							
Dimethyl-	10.64	1		Di-n-butyl-	11.25	1	
Di-n-propyl-	11.00	1		Diisobutyl-	10.50	1	
Diisopropyl-	11.05	1		-Ethylpyrroline	7.43	2	
t-Butylcyclohexyl-	11.23	1		-Benzylpyrroline-	7.08	2	
-Cyclohexylpyrroline	7.95	2		2-Methylpiperidine	10.99	2	
-(p-Tolyl)pyrroline	7.59	2		-Cyclohexylpyrrolidine	10.80	2	
-Ethylpyrrolidine	10.43	2		-(p-Tolyl)pyrrolidine	10.01	2	
-Benzylpyrrolidine	10.36	2		N,O-dimethylhydroxylamine	4.75	12	
N-methylhydroxylamine	5.96	12		Acetanilide	+0.61	4	
Diethyl-	10.98	1		<i>*thermodynamic value</i>			

**Aliphatic Amines**

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

**Secondary Amines**

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

**Tertiary amines**

Trimethyl-	9.76	1
Dimethyldiethyl-	10.29	1
Dimethyl-n-propyl-	9.99	1
Dimethyl-isobutyl-	9.91	1
Dimethyl-sec-butyl-	10.40	1
Tri-n-propyl-	10.65	1
Triallyl-	8.31	1
N-Allylpiperidine	9.69	2

**1-Diethylamino-hexane-thiol-(6)****Cyanoamines**

N-piperidine-CH <sub>2</sub> CN	4.55	8
Et <sub>2</sub> NCN	-2.0	8
Et <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN	7.65	8
Et <sub>2</sub> N(CH <sub>2</sub> ) <sub>4</sub> CN	10.08	8
Et <sub>2</sub> NC(CH <sub>3</sub> ) <sub>2</sub> CN	9.13	8
EtN(CH <sub>2</sub> CN) <sub>2</sub>	-0.6	8
EtN(CH <sub>2</sub> CH <sub>2</sub> CN) <sub>2</sub>	4.55	8
H <sub>2</sub> NCH <sub>2</sub> CN	5.34	8
N-Amphetamine-(CH <sub>2</sub> ) <sub>2</sub> -CN	7.23	8
N-Norcodeine-(CH <sub>2</sub> ) <sub>2</sub> CN	5.68	8
Dimethylcyanamide	1.2	9
Diethylcyanamide	1.2	9
Aminoacetonitrile	5.3	9
Diethylaminoacetonitrile	4.5	9

**Methyl- -diethylamino-ethyl-sulfide**

1,2-Dimethyl- 2-pyrroline	11.94	2
1-methyl-2-n-butyl- 2-pyrroline	11.90	
1-Ethyl-2-methyl- 2-pyrroline	11.92	2
1-n-Butyl-2-methyl- 2-pyrroline	11.90	2
1,2-Dimethyl- 2-tetrahydropyridine	11.57	2
N-Ethyl derivative of: 1,2-Imino-ethane	7.93	7
Trans-2,3-Iminobutane	9.47	7
Trimethylhydroxylamine	3.65	12
Dimethylethyl-	9.99	1
Triethyl-	10.65	1
Dimethyl-n-butyl-	10.02	1
Dimethyl-isopropyl-	10.30	1
Dimethyl-t-butyl-	10.52	1
Tri-n-butyl-	10.89	1
Diallylmethyl-	8.79	1
1-n-Propylpiperidine	10.48	2
10.1	10.1	5
9.8	--	5
1,2-Dimethylpyrrolidine	10.26	2
1-Methyl-2-n-butylpyrrolidin	10.24	2
1-Ethyl-2-methylpyrrolidine	10.64	2
1-n-Butyl-2-methylpyrrolidine	10.43	2
1-Ethyl-2-methylpyrrolidine	10.70	2
1,2-Iminobutane	8.18	7
cis-2,3-Iminobutane	8.56	7
N-dimethylhydroxylamine	5.20	12
Allyldimethyl	8.78	1
1,2-Dimethylpiperidine	10.26	2
1-Ethyl-2-methyl- 2-tetrahydropyridine	11.57	2
2-Amino-2-cyanopropane	5.3	9
-Isopropylaminopropionitrile	8.0	9
-Diethylaminopropionitrile	7.6	9
Et <sub>2</sub> NCH <sub>2</sub> CN	4.55	8
Et <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> CN	9.29	8
Et <sub>2</sub> N(CH <sub>2</sub> ) <sub>5</sub> CN	10.46	8
HN(CH <sub>2</sub> CN) <sub>2</sub>	0.2	8
HN(CH <sub>2</sub> CH <sub>2</sub> CN) <sub>2</sub>	5.26	8
N(CH <sub>2</sub> CH <sub>2</sub> CN) <sub>3</sub>	1.1	8
N-piperidine-C(CH <sub>3</sub> ) <sub>2</sub> CN	9.22	8
N-Methamphetamine-(CH <sub>2</sub> ) <sub>2</sub> CN	6.95	8
Methyl cyanamide	1.2	9
Ethyl cyanamide	1.2	9
Cyanamide	1.1	9
Dimethylaminoacetonitrile	4.2	9

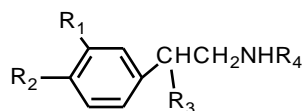
-Aminopropionitrile	7.7	9
-Dimethylaminopropionitrile	7.0	9
, "-Dicyanodiethylamine	5.2	9

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

**Fluoro-substituted amines**

CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	5.7	10
CF <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	4.75	10

CF <sub>3</sub> CH <sub>2</sub> NHCH <sub>3</sub>	6.05	10
<b>Phenylethylamines</b>		
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 <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	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 <sub>3</sub>	10.31
H	H	OH	CH <sub>3</sub>	9.31
H	OH	OH	CH <sub>2</sub>	8.62
OH	H	OH	CH <sub>3</sub>	8.89
H	OH	H	CH <sub>3</sub>	9.36
OH	OH	H	CH <sub>3</sub>	8.78
OH	OH	OH	CH <sub>3</sub>	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	<b>Amines other</b>	
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	<b>Anilines</b>	Ref. 2
Cyclodecyl	9.85	<b>Monosubstituted</b>	
Cycloundecyl	9.71	<b>Substituent</b>	<b>o</b> <b>m</b> <b>p</b>
Cyclododecyl	9.62	H-	4.62* 4.64* 4.58*



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

\*Thermodynamic

**Dimethyl**

H	5.07	52
m-NO <sub>2</sub>	2.63	52
m-CN	2.97	52
p-NO <sub>2</sub>	0.61	52
p-CN	1.78	52
p-NO	4.54	52

**Dimethyl (in 50% ethanol)****Substituent XC<sub>6</sub>H<sub>4</sub>N(CH<sub>3</sub>)<sub>2</sub>** ref. 2

H-	4.21, 4.09
m-CH <sub>3</sub>	4.66
p-C <sub>2</sub> H <sub>5</sub> -	4.69
o-(CH <sub>3</sub> ) <sub>2</sub> CH-	5.05
p-CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -	4.62
o-(CH <sub>3</sub> ) <sub>3</sub> C-	4.26
p-I-	3.43, 2.73
p-Br-	3.52, 2.82
p-Cl-	3.33
m-(CH <sub>3</sub> ) <sub>3</sub> Si-	4.41
o-CH <sub>3</sub> O-	5.49
o-CH <sub>3</sub>	5.15, 5.07
p-CH <sub>3</sub>	4.94
p-CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -	4.43
p-(CH <sub>3</sub> ) <sub>2</sub> CH-	4.77
p-(CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> -	4.19

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

H-	4.25
2-CH <sub>3</sub> -	3.98, 4.09
2,3-(CH <sub>3</sub> ) <sub>2</sub> -	4.42
2,4-(CH <sub>3</sub> ) <sub>2</sub> -	4.61
2,5-(CH <sub>3</sub> ) <sub>2</sub> -	4.17, 4.23
2,6-(CH <sub>3</sub> ) <sub>2</sub> -	3.42, 3.49
3,5-(CH <sub>3</sub> ) <sub>2</sub> -	4.48
2-CH <sub>3</sub> -	4.09
2-(CH <sub>3</sub> ) <sub>2</sub> CH-	4.06
2-(CH <sub>3</sub> ) <sub>2</sub> C-	3.38
2,6-(CH <sub>3</sub> ) <sub>2</sub> -4-(CH <sub>3</sub> ) <sub>3</sub> C-	3.88
2,4-(CH <sub>3</sub> ) <sub>2</sub> -6-(CH <sub>3</sub> ) <sub>3</sub> -	3.43
2-CH <sub>3</sub> -4,6-(CH <sub>3</sub> ) <sub>3</sub> C-	3.31
2,4,6-[(CH <sub>3</sub> ) <sub>3</sub> C <sub>3</sub> ]-	<2

**Substituted Naphthylamines**

1-NH <sub>2</sub> -	3.92*
1-NH <sub>2</sub> -2-NO <sub>2</sub> -	-1.6
1-NH <sub>2</sub> -3-NO <sub>2</sub> -	2.22
1-NH <sub>2</sub> -4-NO <sub>2</sub> -	0.54
1-NH <sub>2</sub> -5-NO <sub>2</sub> -	2.80
1-NH <sub>2</sub> -6-NO <sub>2</sub> -	3.15
1-NH <sub>2</sub> -7-NO <sub>2</sub> -	2.83

1-NH <sub>2</sub> -8-NO <sub>2</sub> -	2.79
1-NH <sub>2</sub> -8-SO <sub>3</sub> -	1.71
1-NH <sub>2</sub> -3-SO <sub>3</sub> -	3.20*
1-NH <sub>2</sub> -4-SO <sub>3</sub> -	2.81*
1-NH <sub>2</sub> -5-SO <sub>3</sub> -	3.69*
1-NH <sub>2</sub> -6-SO <sub>3</sub> -	3.80*
1-NH <sub>2</sub> -7-SO <sub>3</sub> -	3.66
1-NH <sub>2</sub> -8-SO <sub>3</sub> -	5.03*
2-NH <sub>2</sub> -	4.11*
2-NH <sub>2</sub> -1-NO <sub>2</sub> -	-1.0
2-NH <sub>2</sub> -3-NO <sub>2</sub> -	2.93
2-NH <sub>2</sub> -4-NO <sub>2</sub> -	2.63
2-NH <sub>2</sub> -5-NO <sub>2</sub> -	3.16
2-NH <sub>2</sub> -6-NO <sub>2</sub> -	2.75
2-NH <sub>2</sub> -7-NO <sub>2</sub> -	3.13
2-NH <sub>2</sub> -8-NO <sub>2</sub> -	2.86
2-NH <sub>2</sub> -1-SO <sub>3</sub> -	2.35
2-NH <sub>2</sub> -3-SO <sub>3</sub> -	--
2-NH <sub>2</sub> -4-SO <sub>3</sub> -	3.70
2-NH <sub>2</sub> -5-SO <sub>3</sub> -	3.96*
2-NH <sub>2</sub> -6-SO <sub>3</sub> -	3.74*
2-NH <sub>2</sub> -7-SO <sub>3</sub> -	3.95*
2-NH <sub>2</sub> -8-SO <sub>3</sub> -	3.89*

**N-substituted anilines\***

R	C <sub>6</sub> H <sub>5</sub> NHR	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> )R	C <sub>6</sub> H <sub>5</sub> NR <sub>2</sub>	2-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NHR	2-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NR <sub>2</sub>
H-	4.58	4.85	4.58	4.39	4.39
CH <sub>3</sub> -	4.85	5.06	5.06	4.59	5.86
C <sub>2</sub> H <sub>5</sub> -	5.11	5.98	6.56	4.92	7.18
n-C <sub>3</sub> H <sub>7</sub> -	5.02	--	5.59	--	--
n-C <sub>4</sub> H <sub>9</sub> -	4.95	--	~5.7	--	--
i-C <sub>4</sub> H <sub>9</sub> -	--	5.20	--	--	--
sec-C <sub>4</sub> H <sub>9</sub> -	--	6.04	--	--	--
t-C <sub>6</sub> H <sub>12</sub> -	6.30	--	--	--	--
Cyclopentyl-	5.30	6.71	--	5.07	--
Cyclohexyl-	5.60	6.35	--	5.34	--
t-C <sub>4</sub> H <sub>9</sub> -	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

N-Dimethyl-cysteamine	7.95, 10.7
N-Dipropyl-cysteamine	8.00, 10.8
N- -Mercaptoethyl-morpholine	6.65, 9.8
1-Diethylamino-butan- (4)	10.1

Methyl-[ -diethylamino-ethyl]sulfide	9.8
N-Diethyl-cysteamine	7.8, 10.75
N- -Mercaptoethyl-piperidine	7.95, 11.05
1-Diethylamino-propan- (3)	8.0, 10.5
1-Diethylamino-hexan- (6)	10.1

## ANILINES (Ref. 88)

## m-Substituted anilines

m-C <sub>2</sub> H <sub>5</sub>	4.70	m-CH(CH <sub>3</sub> ) <sub>2</sub>	4.67
-C(CH <sub>3</sub> ) <sub>3</sub>	4.66	3,5-(CH <sub>3</sub> ) <sub>2</sub>	4.74
3,5-[C(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub>	4.97	m-COCH <sub>3</sub>	3.56
m-CN	2.76	3-Cl,5-OCH <sub>3</sub>	3.10
3-OCH <sub>3</sub> ,5-NO <sub>2</sub>	2.11	3,5-(OCH <sub>3</sub> ) <sub>2</sub>	3.82
3,5-Br <sub>2</sub>	2.34		

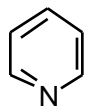
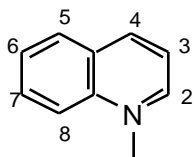
## NAPHTHALAMINES (reference 88)

## substituted naphthalamines

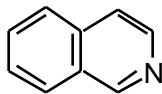
<b>2-naphthalamine</b>	<b>X</b>	4.16	<b>2-naphthalamine</b>	<b>X</b>	
1-NH <sub>2</sub> ,3-X	NO <sub>2</sub>	2.07	2-NH <sub>2</sub> ,4-X	NO <sub>2</sub>	2.43
	CN	2.26		CN	2.66
	Cl	2.66		Cl	3.38
	Br	2.67		Br	3.40
	I	2.82		I	3.41
	COOCH <sub>3</sub>	3.12		COOCH <sub>3</sub>	3.38
	OCH <sub>3</sub>	3.26		OCH <sub>3</sub>	4.05
	OH	3.30	1-NH <sub>2</sub> ,6-X	NO <sub>2</sub>	2.89
	CH <sub>3</sub>	3.96		Cl	3.48
	Cl	2.71		OCH <sub>3</sub>	3.90
2-NH <sub>2</sub> ,5-X	NO <sub>2</sub>	3.01		OH	3.97
	OH	4.07	2-NH <sub>2</sub> ,7-X	NO <sub>2</sub>	3.10
1-NH <sub>2</sub> ,5-X	NO <sub>2</sub>	2.73		Cl	3.71
	OH	3.96		OCH <sub>3</sub>	4.19
	Cl	3.34		OH	4.25
	NH <sub>2</sub>	4.21		NH <sub>2</sub>	4.66
1-NH <sub>2</sub> ,7-X	NO <sub>2</sub>	2.55	2-NH <sub>2</sub> ,6-X	NO <sub>2</sub>	2.62
	Cl	3.48		OCH <sub>3</sub>	4.64
	OCH <sub>3</sub>	4.07	2-NH <sub>2</sub> ,8-X	NO <sub>2</sub>	2.73
	OH	4.20	1-NH <sub>2</sub> ,4-X	NO <sub>2</sub>	0.54
1-NH <sub>2</sub> ,2-X	NO <sub>2</sub>	-1.74		Br	3.21
1-X,2-NH <sub>2</sub>	NO <sub>2</sub>	-0.85	2-NH <sub>2</sub> ,3-X	NO <sub>2</sub>	1.48
1-NH <sub>2</sub> ,8-X	NO <sub>2</sub>	2.79			

<b>Anilines (in 50% ethanol)</b>					
<b>Unhindered</b>	<b>pK</b>	<b>ref.</b>			
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			
<b>Hindered</b>					
o-Aminodiphenyl	3.03	40			
<b>peri</b>					
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			
<b>meso</b>					
9-Anthrylamine	2.7	40			
<b>o-Aminophenols</b>					
3-Hydroxyanthranilic acid	10.09, 5.20	51			
2-Aminophenol hydrochloride	9.99, 4.86	51			
<b>Indicators</b>					
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			
<b>Heterocyclics</b>					
<b>Nucleosides, etc.</b>					
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			

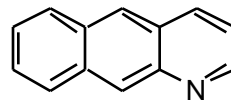
## Heterocyclic Bases (Ref. 2)

Pyridine 5.14\*  
pK (20°)

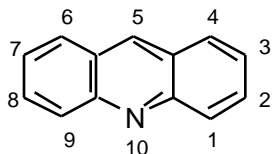
Quinoline 4.85\*



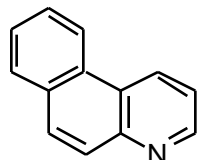
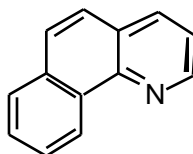
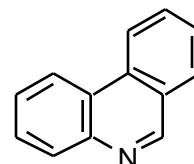
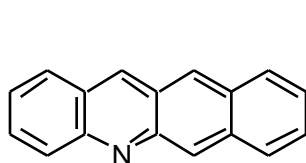
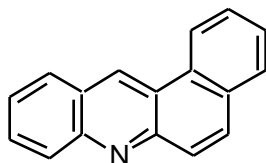
Isoquinoline 5.14\*



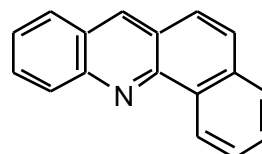
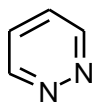
Benzoquinoline 5.05\*



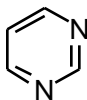
Acridine 5.60

5,6-Benzoquinoline  
5.15\*7,8-Benzoquinoline  
4.25\*Phenanthridine 3.30<sup>a</sup>2,3-Benzacridine 4.52<sup>a</sup>

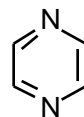
3,4-Benzacridine 4.70\*

1,2-Benzacridine 3.45<sup>a</sup>

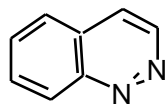
Pyridazine 2.10\*



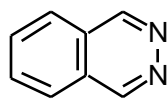
Pyrimidine 1.10\*



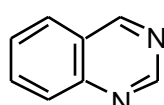
Pyrazine 0.37\*



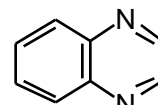
Cinnoline 2.64\*



Phthalazine 3.39\*



Quinazoline 3.31\*



Quinoxaline 0.6\*

<sup>a</sup> 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 <sup>a</sup>			
H <sub>2</sub> N--	4.40*	8.04*	5.88*	6.04*	9.99*
	3.59 <sup>a</sup>	7.61 <sup>a</sup>	5.03 <sup>a</sup>	5.50 <sup>a</sup>	9.45 <sup>a</sup>
HO--	4.18 <sup>a</sup>	4.86 <sup>a</sup>	5.52 <sup>39</sup>	4.45 <sup>a</sup>	-.32 <sup>39</sup>
	10.7 <sup>a</sup>	9.9 <sup>a</sup>	8.81 <sup>39</sup>	9.4*	>12
CH <sub>3</sub> --	3.95 <sup>a</sup>		4.60 <sup>a</sup>		4.70 <sup>a</sup>
H <sub>2</sub> K-(1-CH <sub>3</sub> --)--				4.79 <sup>a</sup>	9.73 <sup>s</sup> 3.22 <sup>a</sup>
1,9-(CH <sub>3</sub> ) <sub>2</sub> --	2.88 <sup>a</sup>				

<sup>a</sup> 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 <sup>a</sup>	19
	40		4-amino-2-methyl-	9.45 <sup>a</sup>	19
3-amino-6,7-benzoquinoline	4.78	40	4-amino-2-methyl-8-chloro-	5.95 <sup>a</sup>	19
8-amino-3,4-benzacridine	7.42	40	8-chloro-	2.5 <sup>a</sup>	19
1'-amino-5,6-benzoquinoline	5.03	40	3,4-diamino-	8.15 <sup>a</sup>	19
4'-amino-5,6-benzoquinoline	5.20	40	3-amino-	4.78, 3.73 <sup>a</sup>	19
2-amino-4-methyl-7,8,benzoquinoline			7,8-benzquinoline	4.25, 3.15 <sup>a</sup>	19
	6.74	40	4-amino-	7.68 <sup>a</sup>	19
6,7-benzoquinoline	5.05, 3.84 <sup>a</sup>	19	4-amino-2-methyl-	7.96 <sup>a</sup>	19
5,6-benzoquinoline	5.15, 3.90 <sup>a</sup>	19	2-amino-4-methyl-	6.74, 6.02 <sup>a</sup>	19
4-amino-	7.99 <sup>a</sup>	19	6-amino-2-methyl-	5.23 <sup>a</sup>	19
2-methyl-	4.44 <sup>a</sup>	19	1'-amino-2-methyl-	4.75 <sup>a</sup>	19
4-amino-2-methyl-	8.45 <sup>a</sup>	19	3,4-benzacridine	4.70, 4.16 <sup>a</sup>	19
2-amino-4-methyl-	7.14, 6.51 <sup>a</sup>	19	5-amino	8.41 <sup>a</sup>	19
4'-amino-	5.20, 4.10 <sup>a</sup>	19	7-amino-	5.03 <sup>a</sup>	19
3'-amino-	4.02 <sup>a</sup>	19	8-amino-	7.42 (6.51) <sup>a</sup>	19
1'-amino-	5.03	19	8-acetamido-	4.48 <sup>a</sup>	19
2',4'-diamino-	4.91 <sup>a</sup>	19	8-dimethylamino-	7.31, 6.99	19
Benziminazole	5.53	19	1,2-benzacridine	3.45 <sup>a</sup>	19
2-amino-	7.54	19	5-amino-	8.13 <sup>a</sup>	19
Benztriazole	1.6	19	7-amino	4.05 <sup>a</sup>	19
Benzthiazole	1.2, 0.1 <sup>a</sup>	19	8-amino-	6.72, 5.97 <sup>a</sup>	19
2-amino-	4.51	19	4',5'-diamino-	8.44 <sup>a</sup>	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 <sup>a</sup>	19	5-hydroxy	7.40, 1.92	39
5-amino-	9.72 <sup>a</sup>	19	7-hydroxy	7.56, 3.31	39
5-acetamido-	4.56 <sup>a</sup>	19	4-methoxy	--, 3.21	39
7-amino-	5.38 <sup>a</sup>	19			
5-amino-6:7:8:9-tetrahydro-	9.66 <sup>a</sup>	19	<b>Heterocyclics</b>		
Caffeine	0.61	4	o,o'-dipyridyl	4.43	6
cinchonine	7.2	4	<b>hydantoin</b>	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	<b>Imidazoles</b>		

2-Methylimidazole	7.75	43	Histidine	methylester	
N-Acetylhistidine	7.05	43		5.2 (NH <sub>2</sub> 7.1)	
2-Methyl-4-hydroxy-aminobenz-	6.65	43		43	
4-Hydroxymethyl-	6.45	43	2-Methyl-4-hydroxy-6-nitro-benzimidazole	3.9	43
2-Methylbenz-	6.1	43			
Histamine	6.0	43	4-Hydroxy-6-Nitrobenz-	3.05	43
4-Hydroxy-6-aminobenz-	5.9	43	b <sup>2</sup> -Hydroxymethylnaphth(1,2)-	4.44, 12.23	86
4-Hydroxybenz-	5.3 (OH 9.5)	43	b <sup>2</sup> -Hydroxymethylnaphth(2,3)-	4.50, 12.23	86
4-Methoxybenz-	5.1	43		4.80, 8.68	44
4-Bromo-	3.7	43	4-Hydroxy-	7.62	40
6-Nitrobenz-	3.05, 10.6	43	1-Amino-	6.28	40
4-Nitro-	1.5, 9.1	43	4-Amino-	7.17	40
<b>isoQuinolines</b>			6-Amino-	6.06	40
1-Hydroxy-	-1.2	44	8-Amino-	5.70	40
5-Hydroxy	5.40, 8.45	44	7-Hydroxy-	3.05	44
3-Amino-	5.05	40	1-Methoxy-	1.35	88
5-Amino-	5.59	40	4-NO <sub>2</sub>	3.31	88
Amino-	6.20	40	4-Br	--, 1.44	39
6-Hydroxy-	5.85, 9.15	44	1-Hydroxy-	--, 4.9	39
8-Hydroxy-	5.66, 8.40	44	5-Methyl-1-phenazone	3.11 <sup>a</sup>	19
2-Methylisoquinolone	-1.8	44	m-Phenanthroline	ca. 7.3, 7.29 <sup>a</sup>	19
Isoquinoline	5.46, 5.14	44, 19	1-Amino-	4.23	19
Phenazine	--, 1.23	39	2,2'-Dipyridyl	8.79, 4.82	44
2-Hydroxy-	7.5, 2.6	39	2-Hydroxy-	4.38, 8.68	44
10-Methyl-2-phenazone	--, 3.0		7-Hydroxy-	--, 2.38	44
6-Aminophenanthridine	6.88	40	9-Methoxy-	5.66 <sup>a</sup>	19
9-Aminophenanthridine	7.31	40	2-Amino-9-methyl-	6.26 <sup>a</sup>	19
o-Phenanthroline	4.27 <sup>a</sup> , 5.2	19	2,7-Diamino-9-methyl-	6.88	40
p-Phenanthroline	3.12 <sup>a</sup>	19	6-Amino-	1.23	19
1,10-Diamino-3,8-Dimethyl-	8.78 <sup>a</sup> , 6.31 <sup>a</sup>		Phenazine	2.6 <sup>a</sup>	19
Phenanthridine	--, 4.65	44	1-Amino-	4.75, 3.46 <sup>a</sup>	19
6-Hydroxy-	8.43, 5.35	44	2-Amino-	5.64 <sup>a</sup>	19
9-Hydroxy (phenanthridone)	<-1.5	44	1,3-Diamino-	4.74	19
9-Amino-	7.31, 6.75 <sup>a</sup>	19	2,3-Diamino-	4.63, 3.9 <sup>a</sup>	19
2,7,9-Triamino-	8.06 <sup>a</sup>	19	2,7-Diamino-	8.26	77
Phthalazine	3.47	19	Pteroylglutamic acid		
1-Amino-	6.60	19	<b>Pyridines</b>		
1-Hydroxy-	11.00, -2	39	2-Amino-	6.86	41
Picolinic acid	5.52	4	4-Amino-	9.17	41
5,5-dimethyl-2-thio-	8.71	42	2-Methyl-	5.94 <sup>b</sup>	45
5,5-Diphenyl-2-thio-	7.69	42	2-Vinyl-	4.98	45
1-Methyl-5,5-pentamethyl-ene-2-thio-	9.25	42	2-Chloro-	0.49	45
4-Methyl-	7.45	43	2,4,6-Trihydroxy-	4.6, 9.0, 13	39
Imidazole	6.95	43	1-Methyl-4-pyridone	3.33	
4-(2',4'-Dihydroxyphenyl)-	6.45	43	2-(N-Methylacetamido)-	2.01	46
Carbobenzoxy-L-histidyl-L-tyrosine ethyl ester	6.25	43	2-Benzamido-	3.33	
6-Aminobenz-	6.0 (NH <sub>2</sub> 3.0)		2-(N-Methylbenzamido)-	1.44	
Benzimidazole	5.4	43	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 <sub>3</sub> ) <sub>2</sub> CH-	5.83 <sup>b</sup>	5.72 <sup>b</sup>	6.02 <sup>b</sup>
4-Benzamido-	5.32	46	CH <sub>3</sub> CO		3.18 <sup>b</sup>	
3-NO <sub>2</sub>	0.81	88	H <sub>2</sub> N-	6.68 <sup>b</sup>	5.80 <sup>b</sup>	8.96 <sup>b</sup>
3-COO <sup>-</sup>	4.77	47	CONH <sub>2</sub> <sup>47</sup>		3.40	3.61
2,3-Me <sub>2</sub>	6.60	48	NC- <sup>47</sup>		1.45	
2,5-Me <sub>2</sub>	6.47	48				
3,4-Me <sub>2</sub>	6.52	48				
2,4,6-Me <sub>3</sub>	7.48	48				
4-OEt	6.67	48				
3-Cl	2.84	48				
3-CO <sub>2</sub> Et	3.35	48				
3-COOH	3.13	88				
2-Amyl-	6.00 <sup>b</sup>	45				
2-Hexyl-	5.95 <sup>b</sup>	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 <sup>-</sup>	4.90	47				
2,4-Me <sub>2</sub>	6.72	48				
2,6-Me <sub>2</sub>	6.77	48				
3,5-Me <sub>2</sub>	6.14	48				
2-Me,5-Et	6.51	48				
3-F	3.10	48				
3-Br	2.84	48				
4-CO <sub>2</sub> Et	3.45	48				

Pyridine N-oxides (see oxygen acids)

### Substituted Pyridines

Pyridine	2-	3-	4-
H-	5.17 <sup>b</sup>		
Cl-	0.72 <sup>b</sup>	2.84 <sup>b</sup>	
I-	1.82 <sup>b</sup>	3.25 <sup>b</sup>	
CH <sub>3</sub> CH <sub>2</sub> -	5.97 <sup>b</sup>	5.70 <sup>b</sup>	6.02 <sup>b</sup>
(CH <sub>3</sub> ) <sub>3</sub> C-	5.76 <sup>b</sup>	5.82 <sup>b</sup>	5.99 <sup>b</sup>
HO-	0.75	4.86	3.27
	11.62	8.72	11.09
SO <sub>3</sub> <sup>-47</sup>		2.9	
CH <sub>3</sub> O-	3.28	4.88	6.62
F-	-0.44 <sup>b</sup>	2.97 <sup>b</sup>	
Br-	0.90 <sup>b</sup>	2.84 <sup>b</sup>	
CH <sub>3</sub> -	5.97 <sup>b</sup>	5.68 <sup>b</sup>	6.02 <sup>b</sup>

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

Substituent	pK	ref.
H-	4.38	2
2-C <sub>2</sub> H <sub>5</sub> -	4.93	2
2-(CH <sub>3</sub> )	4.68	2
2,6-[(CH <sub>3</sub> ) <sub>2</sub> CH] <sub>2</sub>	3.58	2
2-(CH <sub>3</sub> ) <sub>3</sub> C-	4.68	2
2-C <sub>2</sub> H <sub>5</sub> -6-(CH <sub>3</sub> ) <sub>3</sub> C-	4.36	2
2,6-[(CH <sub>3</sub> ) <sub>3</sub> C] <sub>2</sub> <sup>-</sup>	3.58	2
2-CH <sub>3</sub> -	5.05	2
2-(CH <sub>3</sub> ) <sub>2</sub> CH-	4.82	2
2,6-(CH <sub>3</sub> ) <sub>2</sub>	5.77	2
2,6-[(CH <sub>3</sub> ) <sub>3</sub> C] <sub>2</sub>	3.58	2
2-CH <sub>3</sub> -6-(CH <sub>3</sub> ) <sub>3</sub> C	5.52	2
2-(CH <sub>3</sub> ) <sub>2</sub> CH-6-(CH <sub>3</sub> ) <sub>3</sub> 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 <sub>NH</sub>	35°	pK <sub>OH</sub>	
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 <sub>2</sub> 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 <sub>3</sub>	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 <sub>2</sub> C	4.96*	4.62*	4.53*	4.81*	4.98*	4.97*	7.20*	2
NO <sub>2</sub>		1.03 <sup>88</sup>						

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 <sup>a</sup>	19	
2-Amino-	4.43	19	
6-Amino-	3.2 <sup>a</sup>	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 <sup>a</sup>	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 <sup>-</sup>	3.07, 13.25	77
Dithiooxamide (rubeanic acid, H <sub>2</sub> NCSCSNH <sub>2</sub> )	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 <sub>2</sub> ) <sub>2</sub> SH	12.0	13.96	10.75
X(CH <sub>2</sub> ) <sub>4</sub> SH	12.4	13.25	11.50
X(CH <sub>2</sub> ) <sub>3</sub> SH	13.24	11.14	
X(CH <sub>2</sub> ) <sub>5</sub> 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 <sup>a</sup> , 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 <sub>3</sub> CCH <sub>2</sub> -	7.86	32
C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> -	9.43	82
HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> -	9.51	82
CH <sub>2</sub> =CHCH <sub>2</sub> -	9.96	82
n-C <sub>4</sub> H <sub>9</sub> -	10.66	82
t-C <sub>5</sub> H <sub>11</sub> -	11.21	82
C <sub>2</sub> H <sub>5</sub> OCOCH <sub>2</sub> -	7.95	82
C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CH <sub>2</sub> -	9.38	82
HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> -	9.66	82
n-C <sub>3</sub> H <sub>7</sub> -	10.65	82
t-C <sub>4</sub> H <sub>9</sub> -	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]<sub>2</sub>CHR (in 50% dioxane)** (ref. 28)

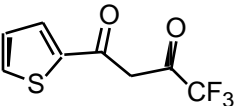
R	R'	R''	pK	pK
CH <sub>3</sub>	CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	11.33	12.52
CH <sub>3</sub>	CH <sub>3</sub>	C <sub>6</sub> H <sub>5</sub>	11.10	12.49
CH <sub>3</sub>	CH <sub>3</sub>	2-ClC <sub>6</sub> H <sub>4</sub>	11.04	12.73
CH <sub>3</sub>	CH <sub>3</sub>	2-C <sub>5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

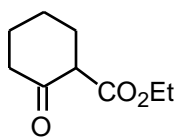
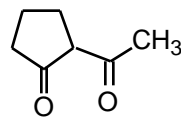
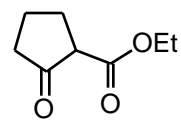
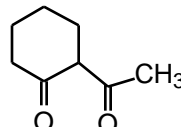
**Bis-(β-Diketones) (RCO)-(R'CO)CH-Y-CH(COR)(COR') (in 50% dioxane)** (ref. 26)

R	R'	Y	pK	pK
CH <sub>3</sub>	CH <sub>3</sub>		9.43	13.54
CH <sub>3</sub>	CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>4</sub>	11.99	12.48
CH <sub>3</sub>	CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>10</sub>	12.01	12.07
CH <sub>3</sub>	CH <sub>3</sub>	1,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub>	11.27	12.15

**Bis-(β-Diketones) RCOCH<sub>2</sub>CO-Y-COCH<sub>2</sub>COR (in 75% dioxane)** (ref. 26)

R	Y	pK	pK
C <sub>6</sub> H <sub>5</sub>	(CH <sub>2</sub> ) <sub>4</sub>	12.47	13.09
C <sub>6</sub> H <sub>5</sub>	(CH <sub>2</sub> ) <sub>5</sub>	12.72	13.46
C <sub>6</sub> H <sub>5</sub>	(CH <sub>2</sub> ) <sub>6</sub>	12.60	13.46
C <sub>6</sub> H <sub>5</sub>	(CH <sub>2</sub> ) <sub>7</sub>	13.1 (est.)	
C <sub>6</sub> H <sub>5</sub>	(CH <sub>2</sub> ) <sub>3</sub>	12.58	13.69
CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>5</sub>	12.29	13.00
CH <sub>3</sub> =CH(CH <sub>3</sub> ) <sub>2</sub>	(CH <sub>2</sub> ) <sub>5</sub>	12.95	13.60

CH <sub>3</sub> NO <sub>2</sub>	10.29	74
CH <sub>3</sub> CHCINO <sub>2</sub>	7	74
CH <sub>3</sub> COCH <sub>2</sub> NO <sub>2</sub>	5.1	74
CH(NO <sub>2</sub> ) <sub>3</sub>	strong	74
CH <sub>3</sub> COCHCl <sub>2</sub>	15	74
CH <sub>3</sub> COCHC <sub>2</sub> H <sub>5</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	12.7	74
CH <sub>3</sub> COCHCH <sub>3</sub> COCH <sub>3</sub>	11	74
CH <sub>3</sub> COCH <sub>2</sub> COC <sub>6</sub> H <sub>5</sub>	9.4	74
C <sub>6</sub> H <sub>5</sub> COCH <sub>2</sub> COCF <sub>3</sub>	6.82	74
CH <sub>3</sub> COCH <sub>2</sub> CHO	5.92	74
CH <sub>3</sub> COCH <sub>2</sub> CO <sub>2</sub> CH <sub>3</sub>	10	74
CH <sub>3</sub> SO <sub>2</sub> CH <sub>2</sub> SO <sub>2</sub> CH <sub>3</sub>	14	74
CH <sub>3</sub> SO <sub>2</sub> CH(COCH <sub>3</sub> ) <sub>2</sub>	4.3	74
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	8.6	74
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> CCH <sub>2</sub> NO <sub>2</sub>	5.82	74
CH <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	3.57	74
CH <sub>3</sub> COCH <sub>2</sub> Cl	c. 16.5	74
CH <sub>3</sub> COCH <sub>2</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	10.68	74
CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	9	74
CH <sub>3</sub> COCHBrCOCH <sub>3</sub>	7	74
CH <sub>3</sub> COCH <sub>2</sub> COCF <sub>3</sub>	4.7	74
C <sub>6</sub> H <sub>5</sub> COCH <sub>2</sub> NC <sub>5</sub> H <sub>5</sub>	10.51	74
CH(COCH <sub>3</sub> ) <sub>3</sub>	5.85	74
CH <sub>3</sub> SO <sub>2</sub> CH <sub>3</sub>	c. 23	74
CH(SO <sub>2</sub> CH <sub>3</sub> ) <sub>3</sub>	strong	74
CH <sub>2</sub> (CN) <sub>2</sub>	11.81	74
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> CCH <sub>2</sub> CN	9	74
CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	~ 24.5	74
CHC <sub>2</sub> H <sub>5</sub> (CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	15	74
CH <sub>3</sub> CONH <sub>2</sub>	~ 25	74
	6.10	74

	10.96	74
	7.82	74
Dinitromethane	4	2
Potassium cyanide	9.21	2
CH(CN) <sub>3</sub>	strong	74
CH <sub>2</sub> (CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	13.3	74
CH <sub>3</sub> CO <sub>2</sub> H	~ 24	74
	10.5	74
	10.1	74
CH <sub>2</sub> (CHO) <sub>2</sub>	5	74
<b>Indicators</b>		
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.