DATA FOR BIOCHEMICAL RESEARCH

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CONTENTS

CONTENTS

TABLE I. 2. CARBOXYLIC ACIDS, ALCOHOLS, ALDEHYDES, AND KETONES

No.	Name	Synonyms	Formula	M. wt.	Physical form	M.p.	B.p.	$[\alpha]_D^t$
8	Acetoacetic acid, Et ester	Ethyl aceto-acetate	$CH_3.CO.CH_2.COOC_2H_5$	130·14	col. liq.	< −80	181	..
9	Acetoin	Acetyl methyl-carbinol	$CH_3.CO.CHOH.CH_3$	88·10	liq.	15	148	..
10	(±)-α-Aceto-lactic acid	..	$CH_3.COH(CO.CH_3).COOH$	132·11	..	..	..	..
11	Acetone	Dimethyl ketone	$CH_3.CO.CH_3$	58·08	col. inflam-mable liq.	−94	56·2	..
12	Acetopyruvic acid	2:4-Dioxo-*n*-valeric acid	$CH_3.CO.CH_2.CO.COOH$	130·10	prisms from benz.	101	130^{37}	..
13	—, Et ester	..	$CH_3.CO.CH_2.CO.COOC_2H_5$	158·15	liq.	18	213–15 117–19[22]	..
14	Aconitic acid, *cis*-	1:2:3-Pro-penetri-carboxylic acid	$HOOC.CH_2.C(COOH)=HC.COOH$	174·11	wh. needles	130	..	..
15	—, —, an-hydride	..	$HOOC.CH_2.C(=CO)-O-HC.CO$	156·09	needles	77	..	..
16	—, *trans*-	..	$HOOC.CH_2.C(COOH)=HOOC.CH$	174·11	needles or leaflets from H_2O	190–210 d.	..	..
17	Adipic acid	Hexanedioic acid	$HOOC.CH_2.CH_2.CH_2.CH_2.COOH$	146·14	col. monocl. prisms from hot HNO_3	153	265^{100}	..
18	Benzoic acid	..	$C_6H_5.COOH$	122·12	monocl. leaflets or needles	122	249	..
19	—, Na salt	..	$C_6H_5.COONa$	144·11	wh. cryst. powder	..	..	..
20	—, K salt	..	$C_6H_5.COOK.3H_2O$	Hydrate, 214·26	wh. cryst. powder	..	..	..
21	2:3-Butane-diol	2:3-Butylene glycol	$CH_3.CHOH.CHOH.CH_3$	90·12	col. liq.	..	182·5	..
22	Butyralde-hyde	Butanal	$CH_3.CH_2.CH_2.CHO$	72·10	col. liq.	−99	75	..
23	*n*-Butyric acid	Butanoic acid	$CH_3.CH_2.CH_2.COOH$	88·10	col. liq.; un-pleasant odour	M.p. −8 F.p. −19	162	..
24	—, Na salt	..	$Na.C_4H_7O_2$	110·10	cryst.	..	..	..
25	—, Ca salt	..	$Ca.(C_4H_7O_2)_2.H_2O$	Hydrate, 232·29	leaflets or prisms	..	..	..
26	*iso*Butyric acid	2-Methyl propanoic acid	$CH_3.CH(CH_3).COOH$	88·10	liq., pungent odour	−47	154·3	..
27	—, Na salt	..	$Na.C_4H_7O_2$	110·10	cryst.	..	..	..
28	—, Ca salt	..	$Ca.(C_4H_7O_2)_2.5H_2O$	Hydrate, 304·35	prisms +5H_2O from cold H_2O	..	..	..
29	Caproic acid	Hexanoic acid	$CH_3.(CH_2)_4.COOH$	116·16	col. oily liq.	−3·9	205	..
30	*iso*Caproic acid	4-Methyl pentanoic acid	$(CH_3)_2CH.CH_2.CH_2.COOH$	116·16	oil	−33	207·7	..
31	Citric acid	2-Hydroxy-1:2:3-pro-panetri-carboxylic acid	$CH_2.COOH.C(OH).COOH.CH_2.COOH$	192·12	monocl. cryst.	153	..	..
32	—, mono-hydrate	..	$C_6H_8O_7.H_2O$	210·14	orthorhom-bic cryst.	Softens 75; melts *ca.* 100	..	..

No.	pKa	Solubility	Preparation	Estimation	General remarks
8	..	$14{\cdot}3^{16\cdot5}$ H_2O; s. EtOH, eth., benz., $CHCl_3$	*Org. Synth.* Coll. 1, 235 (1941)	..	..
9	..	∞ H_2O; v.s. EtOH; i. eth.	*J.B.C.* 191, 401 (1951)	1. *J.B.C.* 161, 495 (1945) 2. *B.B.A.* 8, 18 (1952) 3. *Arch. B.* 9, 229 (1946)	Forms dimer. M.p. 95. Dimer → monomer in aq. soln. (−)-Aceto-ïn, $[\alpha]_D$ −82 approx. Prep. *J.B.C.* 191, 401 (1951).
10	..	s. H_2O	*Arch. B.* 17, 81 (1948)	1. *J.B.C.* 195, 715 (1952) 2. *J.B.C.* 209, 313 (1954)	Obtained only in soln. as Na salt. Natural form is dextrorotatory.
11	..	∞ H_2O, EtOH, eth., most organic solvents	..	1. *J.B.C.* 154, 177 (1944) 2. *J.B.C.* 136, 25 (1940) *B.J.* 51, 218 (1952) 3. *J.B.C.* 176, 501 (1948)	2:4-Dinitrophenylhydrazone, yel. needles from EtOH; M.p. 128.
12	1. 2·61 2. 7·85 (enol)	s. H_2O, EtOH, eth., acet., $CHCl_3$, benz.; i. pet. eth.	*J.B.C.* 175, 573 (1948)	*J.B.C.* 175, 573 (1948)	Stable over long periods as disodium salt. Possesses strong UV absorption due to keto-enol tautomerism. See *J.B.C.* 175, 573 (1948).
13	..	..	*Org. Synth.* Coll. 1, 238 (1941)	..	Absorbs in UV due to enolization. λ_{max} 290 mμ.
14	..	..	*B.J.* 38, 426 (1944)	1. *Anal. Chem.* 24, 1064 (1952) 2. *B.J.* 52, 527 (1952) 3. *B.J.* 38, 426 (1944)	Stable at least 3 months at room temp. Stability in soln., *see B.J.* 38, 426 (1944).
15	..	..	*Ber.* 61, 2521 (1928)	..	Salts usually prepared by neutralization of anhydride.
16	1. 2·80 2. 4·46	18 H_2O; 50·88% EtOH; sl. s. eth.	*Org. Synth.* Coll. 2, 12 (1943)	1. *Anal. Chem.* 24, 1064 (1952) 2. *B.J.* 52, 527 (1952)	..
17	1. 4·42 2. 5·62	1·5 H_2O; s. EtOH; 0·6 eth.; s. HNO_3; i. benz.	*Org. Synth.* Coll. 1, 18 (1941)	..	Recrystallized from conc. HNO_3.
18	4·19	$0{\cdot}29^{20}$, $6{\cdot}8^{95}$ H_2O; 47·1[15], 66[78] EtOH; 40[15] eth.; 22 $CHCl_3$	..	*B.J.* 48, 216 (1951)	Starts to sublime at 100°.
19	..	66^{20}, $74{\cdot}2^{100}$ H_2O; $1{\cdot}64^{25}$, $8{\cdot}3^{78}$ EtOH	..	..	Aq. soln. slightly alkaline (pH about 8).
20	..	52^{25}, 112^{100} H_2O; s. EtOH	..	..	Loses H_2O at 110°.
21	..	∞ H_2O, EtOH	..	*B.B.A.* 8, 18 (1952)	..
22	..	3·7 H_2O; ∞ EtOH, eth.	..	*Organic Analysis* 1, 243 (1953)	2:4-Dinitrophenylhydrazone, cryst. from EtOH; M.p. 123.
23	4·82	∞ H_2O, EtOH, eth.	..	1. *B.J.* 50, 679 (1952) *B.J.* 58, 670 (1954) 2. *See* volatile fatty acids	Volatile in steam.
24	..	s. H_2O; sl. s. EtOH	..	..	..
25	..	Anhyd. salt, 20·3[0], 18·2[20], 15·0[65], 14·0[75], 15·85[100] H_2O. Solubility reaches a minimum at 75°	..	..	..
26	4·85	20 H_2O; ∞ EtOH, eth., $CHCl_3$	..	1. *B.J.* 50, 679 (1952) *B.J.* 58, 670 (1954) 2. *See* volatile fatty acids	Salts are more soluble in H_2O than those of *n*-butyric acid.
27	..	s. H_2O; sl. s. EtOH	..	..	..
28	..	Anhyd. salt, 20·1[0], 23·1[25], 28·7[82], 27·0[80], 26·1[100] H_2O. Solubility reaches maximum at 62·5°	..	..	From hot aq. soln. crystallizes as $Ca(C_4H_7O_2)_2.H_2O$. Transition point 62·5°.
29	4·83	$0{\cdot}97^{20}$, $1{\cdot}17^{60}$ H_2O; s. EtOH, eth.	..	1. *B.J.* 50, 679 (1952) *B.J.* 58, 670 (1954) 2. *See* volatile fatty acids	..
30	4·82	sl. s. H_2O; s. EtOH, eth.	..	1. *B.J.* 50, 679 (1952) *B.J.* 58, 670 (1954) 2. *See* volatile fatty acids	..
31	1. 3·09 2. 4·75 3. 5·41	146^{20}, 525^{100} H_2O; 62^{25} EtOH; 2·25[15] eth. (*see* general remarks)	..	1. *B.J.* 45, 377 (1949) *J.B.C.* 175, 745 (1948) *Anal. Chem.* 23, 467 (1951) *B.J.* 60, 647 (1955) 2. *J.B.C.* 175, 849 (1948)	The solubilities are calculated in terms of the anhyd. compound although below 35·8° the monohydrate is the stable form.
32	..	As for anhyd. citric acid	..	..	Loses H_2O at 70–75° or by standing over conc. H_2SO_4 in a desicator.

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