Butanedioic acid

Other names:	1,2-Ethanedicarboxylic acid
	1,4-Butanedioic acid
	Acid of amber
	Amber acid
	Asuccin
	Bernsteinsaure
	Dihydrofumaric acid
	Ethanedicarboxylic acid
	Ethylene succinic acid
	Katasuccin
	Kyselina jantarova
	NSC 106449
	Sal succini
	Salt of amber
	Succinellite
	Succinic acid
	Wormwood
	Wormwood acid
Inchi:	InChI=1S/C4H6O4/c5-3(6)1-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)
InchiKey:	KDYFGRWQOYBRFD-UHFFFAOYSA-N
Formula:	C4H6O4
SMILES:	O=C(O)CCC(=O)O
Mol. weight [g/mol]:	118.09
CAS:	110-15-6

Physical Properties

Property code	Value	Unit	Source
chs	-1491.20 ± 0.30	kJ/mol	NIST Webbook
chs	-1490.80 ± 0.50	kJ/mol	NIST Webbook
chs	-1491.10 ± 4.10	kJ/mol	NIST Webbook
chs	-1491.30 ± 0.20	kJ/mol	NIST Webbook
chs	-1490.90 ± 0.30	kJ/mol	NIST Webbook
chs	-1491.50 ± 0.50	kJ/mol	NIST Webbook
chs	-1495.00 ± 2.00	kJ/mol	NIST Webbook
chs	-1490.70 ± 0.40	kJ/mol	NIST Webbook
chs	-1490.80 ± 0.30	kJ/mol	NIST Webbook
chs	-1490.80 ± 0.63	kJ/mol	NIST Webbook

chs	-1490.50 ± 0.40	kJ/mol	NIST Webbook
chs	-1489.00 ± 0.30	kJ/mol	NIST Webbook
chs	-1492.80 ± 1.30	kJ/mol	NIST Webbook
chs	-1487.00	kJ/mol	NIST Webbook
chs	-1492.50 ± 0.40	kJ/mol	NIST Webbook
chs	-1491.20 ± 0.19	kJ/mol	NIST Webbook
dm	2.20	debye	KDB
gf	-548.68	kJ/mol	Joback Method
hf	-655.51	kJ/mol	Joback Method
hfs	-940.10 ± 4.20	kJ/mol	NIST Webbook
hfs	-941.00 ± 0.30	kJ/mol	NIST Webbook
hfs	-940.86 ± 0.50	kJ/mol	NIST Webbook
hfs	-940.20 ± 0.20	kJ/mol	NIST Webbook
hfs	-940.35 ± 0.54	kJ/mol	NIST Webbook
hfs	-939.00 ± 0.40	kJ/mol	NIST Webbook
hfs	-938.70 ± 1.30	kJ/mol	NIST Webbook
hfus	34.00	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	121.80 ± 3.30	kJ/mol	NIST Webbook
hsub	118.00 ± 3.00	kJ/mol	NIST Webbook
hsub	123.10	kJ/mol	NIST Webbook
hsub	120.30 ± 4.40	kJ/mol	NIST Webbook
hvap	94.40	kJ/mol	NIST Webbook
log10ws	-0.20		Aqueous Solubility Prediction Method
logp	-0.064		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	6590.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
ss	175.70	J/mol×K	NIST Webbook
ss	167.32	J/mol×K	NIST Webbook
tb	508.00	K	KDB
tc	758.96	K	Joback Method
tf	460.23	K	Aqueous Solubility Prediction Method
tf	458.65	K	Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or n-butanol Mixture
tf	461.00	K	Solubility of Butanedioic Acid in Different Solvents at Temperatures between 283 K and 333 K
tf	456.00	K	KDB

tf	457.44	K	Determination and Thermodynamic Modeling of Solid-Liquid Phase Equilibrium for Succinic Acid in the Glutaric Acid + Adipic Acid + Ethyl Acetate Mixture and Adipic Acid in the Succinic Acid + Glutaric Acid + Ethyl Acetate Mixture
tt	461.00 ± 0.30	K	NIST Webbook
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.00	J/mol×K	583.02	Joback Method
cpg	194.18	J/mol×K	612.34	Joback Method
cpg	199.11	J/mol×K	641.67	Joback Method
cpg	203.80	J/mol×K	670.99	Joback Method
cpg	208.24	J/mol×K	700.31	Joback Method
cpg	212.44	J/mol×K	729.63	Joback Method
cpg	216.41	J/mol×K	758.96	Joback Method
cps	152.93	J/mol×K	298.15	NIST Webbook
cps	164.00	J/mol×K	323.00	NIST Webbook
cps	149.80	J/mol×K	289.80	NIST Webbook
dvisc	0.0000600	Pa×s	583.02	Joback Method
dvisc	0.0026753	Pa×s	394.12	Joback Method
dvisc	0.0009598	Pa×s	431.90	Joback Method
dvisc	0.0092675	Pa×s	356.34	Joback Method
dvisc	0.0001953	Pa×s	507.46	Joback Method
dvisc	0.0001039	Pa×s	545.24	Joback Method
dvisc	0.0004061	Pa×s	469.68	Joback Method
hfust	32.95	kJ/mol	457.00	NIST Webbook
hfust	34.00	kJ/mol	455.20	NIST Webbook
hfust	32.95	kJ/mol	457.00	NIST Webbook
hfust	32.95	kJ/mol	457.00	NIST Webbook
hsubt	128.00 ± 2.00	kJ/mol	338.00	NIST Webbook
hsubt	119.50	kJ/mol	291.00	NIST Webbook
hsubt	120.50	kJ/mol	366.00	NIST Webbook
hsubt	118.10 ± 3.30	kJ/mol	386.50	NIST Webbook
hsubt	73.60	kJ/mol	306.00	NIST Webbook
sfust	72.09	J/mol×K	457.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.96942e+02
Coeff. B	-2.08066e+04
Coeff. C	-2.50252e+01
Coeff. D	7.38328e-06
Temperature range (K), min.	461.15
Temperature range (K), max.	806.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Binary and ternary solid-liquid phase equilibrium for the systems formed by succinic acid, urea and diethylene glycol: Determination and modelling:	https://www.doi.org/10.1016/j.jct.2017.01.010
Solubility of Butanedioic Acid in Different Solvents at Temperatures between 283 K and 333 K:	https://www.doi.org/10.1021/je900021g
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=963
Solid Liquid Phase Equilibrium and Phase Diagram for the Ternary Carbamazepine Succinic Acid Ethanol or Acetone System at (298.15 and 308.15) K:	https://www.doi.org/10.1021/je100918d
Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:	https://www.doi.org/10.1016/j.jct.2004.12.011
Solid Liquid Equilibrium and Phase Diagram for the Ternary Succinic Acid + Glutaric Acid + Water System:	https://www.doi.org/10.1021/je5003785
Solubility of succinic acid in different aqueous solvent mixtures: Experimental measurement and thermodynamic modelling:	https://www.doi.org/10.1016/j.fluid.2012.12.018
Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid and Succinic Acid in Acetic Acid + Cyclohexanone Mixtures:	https://www.doi.org/10.1021/acs.jced.6b00800
Determination and Correlation of Solubilities for Succinic Acid in the Adipic Acid + Glutaric Acid + Acetone Mixture and Adipic Acid in the Succinic Acid + Glutaric Acid + Acetone Mixture:	https://www.doi.org/10.1021/acs.jced.6b00145
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Surface Tensions and Densities of Oxalic, Malonic, Succinic, Maleic, Malic, and cis-Pinonic Acids:	https://www.doi.org/10.1021/je050366x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach:	https://www.doi.org/10.1016/j.jct.2017.09.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110156&Units=SI
Solubilities of Succinic Acid in Acetic Acid + Water Mixtures and Acetic Acid + Cyclohexane Mixtures:	https://www.doi.org/10.1021/je500231c
Solubility Determination and Correlation of Glibenclamide in 11 Monosolvents and (Acetone + Acetonitrile) Binary Solvents from 283.15 K to 323.15 K:	https://www.doi.org/10.1021/acs.jced.8b00717
Determination and Thermodynamic Modeling of Solid-Liquid Phase Equilibrium for Succinic Acid in the Glutaric Acid + Adipic Acid + Ethyl Acetate Mixture and Adipic Acid in the Succinic Acid + Glutaric Acid + Ethyl Acetate Mixture:	https://www.doi.org/10.1021/acs.jced.8b01127
Determination and Correlation of Solid Liquid Phase Equilibrium and Phase Diagram for a Multicomponent System of Mixed Dibasic Acids. Ternary System of Succinic Acid + Adipic Acid + Ethanol:	https://www.doi.org/10.1021/acs.jced.6b00031
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=963
Calibration and test of an aneroid mini-bomb combustion calorimeter:	https://www.doi.org/10.1016/j.jct.2006.10.013
Measurement and Correlation for Solubilities of Succinic Acid and Glutaric Acid in ε-Caprolactone + Acetic Acid Mixtures and ε-Caprolactone + Cyclohexanone Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00660
Solubility of succinic acid, glutaric acid and adipic acid in propionic acid + epsilon-caprolactone + water mixtures: Experimental measurement and thermodynamic modeling:	https://www.doi.org/10.1016/j.jct.2019.06.033

Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or 1-Butanol Mixture:	https://www.doi.org/10.1021/je500682v
Effects of Different Organic Acids on Solubility and Metastable Zone Width of Zinc Lactate:	https://www.doi.org/10.1021/je3006453
Synthesis and Solubility of 5,5-Dimethyl-2-(phenyl(phenylamino)methyl)-1,3,2-dioxaphosphinane 2-oxide in Selected Solvents between 278.15 K and 347.15 K:	https://www.doi.org/10.1021/acs.jced.7b00585
Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid + Dimethyl Adipate + Methanol Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00255
Micro-combustion calorimetry employing a Calvet heat flux calorimeter:	https://www.doi.org/10.1016/j.jct.2004.04.002
Ternary Phase Diagram for Systems of Succinic Acid + Urea + Water, Glutaric Acid + Urea + Water, and Adipic Acid + Urea + Water at 288.15 K and 303.15 K:	https://www.doi.org/10.1021/je500725e
Determination and Correlation for the Solubilities of Succinic Acid in Cyclohexanol + Cyclohexanone + Cyclohexane Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00956
Effect of cyclohexanone on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Determination and correlation of solid-liquid phase equilibrium and phase diagram for multicomponent systems containing dibasic acids. (II) Ternary system of succinic acid + glutaric acid + ethanol system:	https://www.doi.org/10.1016/j.jct.2016.12.010
Measurement and Correlation for the Solubility of Adipic Acid and Succinic Acid in Ethanol + Cyclohexanone Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00468
Critical temperatures and pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume