

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	-1490.90 ± 0.30	kJ/mol	NIST Webbook
chs	-1492.80 ± 1.30	kJ/mol	NIST Webbook
chs	-1491.50 ± 0.50	kJ/mol	NIST Webbook
chs	-1491.30 ± 0.20	kJ/mol	NIST Webbook
chs	-1490.80 ± 0.50	kJ/mol	NIST Webbook
chs	-1491.10 ± 4.10	kJ/mol	NIST Webbook
chs	-1490.50 ± 0.40	kJ/mol	NIST Webbook
chs	-1487.00	kJ/mol	NIST Webbook
chs	-1491.20 ± 0.30	kJ/mol	NIST Webbook
chs	-1489.00 ± 0.30	kJ/mol	NIST Webbook

chs	-1490.80 ± 0.63	kJ/mol	NIST Webbook
chs	-1490.80 ± 0.30	kJ/mol	NIST Webbook
chs	-1490.70 ± 0.40	kJ/mol	NIST Webbook
chs	-1491.20 ± 0.19	kJ/mol	NIST Webbook
chs	-1495.00 ± 2.00	kJ/mol	NIST Webbook
chs	-1492.50 ± 0.40	kJ/mol	NIST Webbook
dm	2.20	debye	KDB
gf	-548.68	kJ/mol	Joback Method
hf	-655.51	kJ/mol	Joback Method
hfs	-940.20 ± 0.20	kJ/mol	NIST Webbook
hfs	-941.00 ± 0.30	kJ/mol	NIST Webbook
hfs	-940.10 ± 4.20	kJ/mol	NIST Webbook
hfs	-938.70 ± 1.30	kJ/mol	NIST Webbook
hfs	-940.86 ± 0.50	kJ/mol	NIST Webbook
hfs	-940.35 ± 0.54	kJ/mol	NIST Webbook
hfs	-939.00 ± 0.40	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	118.00 ± 3.00	kJ/mol	NIST Webbook
hsub	120.30 ± 4.40	kJ/mol	NIST Webbook
hsub	123.10	kJ/mol	NIST Webbook
hsub	121.80 ± 3.30	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.44	J/mol×K	729.63	Joback Method
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	216.41	J/mol×K	758.96	Joback Method
cps	149.80	J/mol×K	289.80	NIST Webbook
cps	152.93	J/mol×K	298.15	NIST Webbook
cps	164.00	J/mol×K	323.00	NIST Webbook
dvisc	0.0000600	Paxs	583.02	Joback Method
dvisc	0.0092675	Paxs	356.34	Joback Method
dvisc	0.0026753	Paxs	394.12	Joback Method
dvisc	0.0009598	Paxs	431.90	Joback Method
dvisc	0.0004061	Paxs	469.68	Joback Method
dvisc	0.0001953	Paxs	507.46	Joback Method
dvisc	0.0001039	Paxs	545.24	Joback Method
hfust	32.95	kJ/mol	457.00	NIST Webbook
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
hsubt	73.60	kJ/mol	306.00	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
sfust	72.09	J/mol×K	457.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

KDB: <https://www.thermo.com/resources/kdb/hcprop/showprop.php?cmpid=963>

Determination and Correlation for the Solubilities of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/acs.jced.7b00956>

Solubilities of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/je500682v>

Solubilities of Succinic Acid, Glutaric Acid, and Adipic Acid in Propionic Acid + Methyl Cellosolve Mixtures: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1016/j.jct.2019.06.033>

Solubilities of Succinic Acid, Glutaric Acid, and Adipic Acid in Propionic Acid + Methyl Cellosolve Mixtures: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1021/acs.jced.7b00255>

Solubilities of Succinic Acid, Glutaric Acid, and Adipic Acid in Propionic Acid + Methyl Cellosolve Mixtures: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1021/je5003785>

Solubilities of Succinic Acid and Glutaric Acid in Water: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1021/acs.jced.7b00660>

Solubilities of Succinic Acid and Glutaric Acid in Water: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1021/acs.jced.7b00585>

5-(Dimethyl((phenyl(phenylamino)methyl)-1,3,2-dioxaphosphinane-2-ylidene)oxy)phosphorothioic acid: Synthesis, Crystal Structure, and Solubility in Organic Solvents. <https://www.doi.org/10.1016/j.fluid.2012.12.018>

Experimental Determination of the Solubility of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/je050366x>

Solubilities of Succinic Acid, Glutaric Acid, and Adipic Acid in Propionic Acid + Methyl Cellosolve Mixtures: Measurement and Correlation for Solid-Liquid Phase Equilibrium. <https://www.doi.org/10.1016/j.jct.2017.09.007>

Determination and Correlation of Solid-Liquid Phase Equilibrium and Phase Diagrams for a Multicomponent System of Solid-Liquid Phase Equilibrium and Phase Diagrams for a Multicomponent System of Solid-Liquid Phase Equilibrium and Phase Diagrams. <https://www.doi.org/10.1021/acs.jced.6b00031>

Determination and Correlation of Solid-Liquid Phase Equilibrium and Phase Diagrams for a Multicomponent System of Solid-Liquid Phase Equilibrium and Phase Diagrams. <https://www.doi.org/10.1016/j.jct.2016.12.010>

Solubility and Phase Diagrams of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/je3006453>

Solubility and Phase Diagrams of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/acs.jced.8b01127>

Modeling of Solid-Liquid Phase Equilibrium for Succinic Acid in the Correlation of Glutaric Acid, n-Propylamine, and n-Propylamine + Succinic Acid in the Correlation of Glutaric Acid, n-Propylamine, and n-Propylamine + Succinic Acid. <https://www.doi.org/10.1021/acs.jced.8b00717>

Solubility and Phase Diagrams of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1016/j.jct.2017.01.010>

Solubility and Phase Diagrams of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. <https://www.doi.org/10.1021/je500725e>

Solubility and Phase Diagrams of Succinic Acid in Organic Solvents: Acetic Acid, Ethyl Acetate, Propyl Acetate, n-Butanol, Methyl Cellosolve, and Dimethyl Sulfoxide. https://en.wikipedia.org/wiki/Joback_method

Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid in Acetic Acid + Cyclohexanone Mixtures: Aqueous Solubility Prediction Method. <https://www.doi.org/10.1021/acs.jced.6b00800>

NIST WebBook. <http://webbook.nist.gov/cgi/cbook.cgi?ID=C110156&Units=SI>

An odd-even effect on solubility of dicarboxylic acids in organic solvents: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

<https://www.doi.org/10.1016/j.jct.2014.05.009>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=963
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Micro-combustion calorimetry employing a Calvet heat flux	https://www.doi.org/10.1016/j.jct.2004.04.002
Calibration Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids	https://www.doi.org/10.1021/je0498356
Solid-Liquid Phase Equilibrium and Phase Diagram for the Ternary System of Succinic Acid, Acetic Acid, and Ethanol	https://www.doi.org/10.1016/j.jct.2006.10.013
Micro-combustion calorimetry: Determination and Correlation of Solubilities for Succinic Acid in the Solubility of Succinic Acid in Acetone	https://www.doi.org/10.1021/acs.jced.6b00145
Differential Scanning Calorimetry: Measurement and Correlation for the Solubility of Adipic Acid and Succinic Acid in Ethanol and Acetone	https://www.doi.org/10.1021/je900021g
Solubility of Succinic Acid in Acetic Acid-Water Mixtures and Acetic Acid-Water Mixtures	https://www.doi.org/10.1021/acs.jced.7b00468
Sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:	https://www.doi.org/10.1021/je500231c
	https://www.doi.org/10.1016/j.jct.2004.12.011

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

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