Hexanedioic acid

Other names:	1,4-Butanedicarboxylic acid
	1,6-Hexanedioic acid
	Acifloctin
	Acinetten
	Adi-pure
	Adilactetten
	Adipic acid
	Adipinic acid
	Hexanedioc acid
	Kyselina adipova
	NSC 7622
	asapic
	inipol DS
Inchi:	InChI=1S/C6H10O4/c7-5(8)3-1-2-4-6(9)10/h1-4H2,(H,7,8)(H,9,10)
InchiKey:	WNLRTRBMVRJNCN-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	O=C(O)CCCCC(=O)O
Mol. weight [g/mol]:	146.14
CAS:	124-04-9

Physical Properties

Property code	Value	Unit	Source
chs	-2768.70 ± 5.90	kJ/mol	NIST Webbook
chs	-2802.40 ± 1.40	kJ/mol	NIST Webbook
chs	-2795.90 ± 0.75	kJ/mol	NIST Webbook
chs	-2791.98 ± 0.42	kJ/mol	NIST Webbook
gf	-531.84	kJ/mol	Joback Method
hf	-696.79	kJ/mol	Joback Method
hfs	-998.22 ± 0.42	kJ/mol	NIST Webbook
hfs	-1021.32	kJ/mol	NIST Webbook
hfus	38.00	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hfus	33.70	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	129.00 ± 1.00	kJ/mol	NIST Webbook

hsub	133.60 ± 1.30	kJ/mol	NIST Webbook
hvap	105.20	kJ/mol	NIST Webbook
log10ws	-0.82		Aqueous Solubility Prediction Method
logp	0.716		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	3850.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
rinpol	1372.40		NIST Webbook
rinpol	1372.40		NIST Webbook
ripol	2137.00		NIST Webbook
tb	628.78	K	Joback Method
tc	802.60	K	Joback Method
tf	424.26	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
tf	425.50 ± 0.30	K	NIST Webbook
tf	425.50 ± 0.30	K	NIST Webbook
tf	425.50 ± 0.40	K	NIST Webbook
tf	425.50 ± 0.30	K	NIST Webbook
tf	426.00 ± 1.50	K	NIST Webbook
tf	425.50 ± 0.50	K	NIST Webbook
tf	425.50 ± 0.30	K	NIST Webbook
tf	422.40 ± 1.00	K	NIST Webbook
tf	430.00 ± 2.00	K	NIST Webbook
tf	424.00 ± 1.50	K	NIST Webbook
tf	426.07 ± 0.20	K	NIST Webbook
tf	425.15	K	Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or n-butanol Mixture
tf	425.50	K	Solubilities of Adipic Acid in Cyclohexanol + Cyclohexanone Mixtures and Cyclohexanone + Cyclohexane Mixtures
tf	425.95	K	Aqueous Solubility Prediction Method
tf	422.00 ± 8.00	K	NIST Webbook
tt	424.70 ± 0.30	K	NIST Webbook
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.81	J/mol×K	802.60	Joback Method
cpg	277.53	J/mol×K	628.78	Joback Method
cpg	284.57	J/mol×K	657.75	Joback Method
cpg	291.27	J/mol×K	686.72	Joback Method
cpg	297.63	J/mol×K	715.69	Joback Method
cpg	303.67	J/mol×K	744.66	Joback Method
cpg	309.39	J/mol×K	773.63	Joback Method
dvisc	0.0000378	Pa×s	628.78	Joback Method
dvisc	0.0058569	Pa×s	378.88	Joback Method
dvisc	0.0016670	Pa×s	420.53	Joback Method
dvisc	0.0005951	Pa×s	462.18	Joback Method
dvisc	0.0002519	Pa×s	503.83	Joback Method
dvisc	0.0001216	Pa×s	545.48	Joback Method
dvisc	0.0000651	Pa×s	587.13	Joback Method
hfust	34.85	kJ/mol	426.40	NIST Webbook
hfust	34.85	kJ/mol	425.50	NIST Webbook
hfust	33.70	kJ/mol	419.00	NIST Webbook
hfust	34.85	kJ/mol	426.40	NIST Webbook
hsubt	129.30 ± 2.50	kJ/mol	382.50	NIST Webbook
hsubt	125.00 ± 20.00	kJ/mol	363.00	NIST Webbook
hsubt	145.00 ± 4.00	kJ/mol	348.00	NIST Webbook
hsubt	146.20	kJ/mol	296.00	NIST Webbook
hsubt	140.00	kJ/mol	306.50	NIST Webbook
hvapt	92.00	kJ/mol	521.50	NIST Webbook
sfust	81.92	J/mol×K	425.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	538.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76921e+01
Coeff. B	-6.86994e+03
Coeff. C	-8.46730e+01
Temperature range (K), min.	479.40
Temperature range (K), max.	639.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.33029e+02
Coeff. B	-1.71566e+04
Coeff. C	-1.58264e+01
Coeff. D	3.22958e-06
Temperature range (K), min.	425.50
Temperature range (K), max.	611.15

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=965
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation for the Solubility of Adipic Acid and Succinic Acid in Glutaric Acid + Cyclohexanone and Glutaric Acid + Acetic Acid Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00468
Viscosity B Coefficients and Activation Parameters of Viscous Flow for Adipic Acid in Aqueous Dextran Solution:	https://www.doi.org/10.1021/je060189f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Thermal analysis of phase change materials in the temperature range 200-300°C:	https://www.doi.org/10.1016/j.tca.2010.11.011
Solubility and thermodynamics of vitamin C in binary liquid mixtures involving water, methanol, ethanol and isopropanol at different temperatures:	https://www.doi.org/10.1016/j.jct.2018.02.005
Determination and correlation of solid-liquid phase equilibrium and phase diagram for multicomponent system of mixed dibasic acids. (I) Ternary system of adipic acid + glutaric acid + methanol:	https://www.doi.org/10.1016/j.fluid.2015.09.036
Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid in Dimethyl Adipate + Methanol Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00255
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
Solubility of Adipic Acid in Acetone, Chloroform, and Toluene:	https://www.doi.org/10.1021/je8006887
Determination and modeling of binary and ternary solid-liquid phase equilibrium for the systems formed by adipic acid, urea and diethylene glycol:	https://www.doi.org/10.1016/j.fluid.2015.12.026
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124049&Units=SI
Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or n-Butanol Mixtures:	https://www.doi.org/10.1021/je500682v
Solubilities of Adipic Acid in Acetic Acid + Water Mixtures and Acetic Acid + Cyclohexane Mixtures:	https://www.doi.org/10.1021/je301202v
Measurement and Correlation for Solubilities of Adipic Acid in Acetic Acid + e-Caprolactone Mixtures and Cyclohexanone + e-Caprolactone Mixtures:	https://www.doi.org/10.1021/acs.jced.6b00177
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of Adipic Acid in Cyclohexanol + Cyclohexanone Mixtures and Cyclohexanone + Cyclohexane Mixtures:	https://www.doi.org/10.1021/acs.jced.5b00880
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Measurement on the solubility of adipic acid in various solvents at high temperature and its thermodynamics parameters:	https://www.doi.org/10.1016/j.fluid.2013.10.003
Solubilities of adipic acid in binary cyclohexanone + cyclohexanol, cyclohexane + cyclohexanol, and cyclohexane + cyclohexanone solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2016.01.006
DIPPR Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=965
An odd-even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
Solid Liquid Equilibrium and Phase Diagram for the Ternary Succinic Acid + Glutaric Acid + Water System:	https://www.doi.org/10.1021/je5003785
Determination and Correlation of Solubilities for Succinic Acid in the Adipic Acid + Glutaric Acid + Acetone Mixture:	https://www.doi.org/10.1021/acs.jced.6b00145
Solubility of succinic acid, glutaric acid and adipic acid in propionic acid + acetone mixtures:	https://www.doi.org/10.1016/j.jct.2019.06.033
Chemical Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Experimental measurement and thermodynamic modeling of Solid-Liquid Phase Equilibrium Involving Xylose, Water, and Ethylene Glycol or 1,2-Propylene Glycol at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.8b01128

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume