Pentanedioic acid

Other names:	1,3-Propanedicarboxylic acid
	1,5-Pentanedioic acid
	Glutaric acid
	Pentandioic acid
Inchi:	InChI=1S/C5H8O4/c6-4(7)2-1-3-5(8)9/h1-3H2,(H,6,7)(H,8,9)
InchiKey:	JFCQEDHGNNZCLN-UHFFFAOYSA-N
Formula:	C5H8O4
SMILES:	O=C(O)CCCC(=O)O
Mol. weight [g/mol]:	132.11
CAS:	110-94-1

Physical Properties

Property code	Value	Unit	Source
chs	-2150.90 ± 1.20	kJ/mol	NIST Webbook
chs	-2150.35 ± 0.75	kJ/mol	NIST Webbook
chs	-2151.60 ± 0.50	kJ/mol	NIST Webbook
gf	-540.26	kJ/mol	Joback Method
hf	-676.15	kJ/mol	Joback Method
hfs	-960.00 ± 1.20	kJ/mol	NIST Webbook
hfs	-960.50 ± 1.10	kJ/mol	NIST Webbook
hfus	2.30	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hfus	21.53	kJ/mol	Solid Liquid Equilibria for Six Binary Mixtures of Pentanedioic Acid, Octanedioic Acid, 3-Methylheptanedioic Acid, 2,2-Dimethylbutanedioic Acid, and 2,3-Dimethylbutanedioic Acid
hfus	21.01	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hsub	119.80 ± 1.20	kJ/mol	NIST Webbook

hvap	101.60	kJ/mol	NIST Webbook
log10ws	1.00		Aqueous Solubility Prediction Method
logp	0.326		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4270.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	605.90	K	Joback Method
tc	780.63	K	Joback Method
tf	369.80 ± 0.60	K	NIST Webbook
tf	371.00 ± 0.40	K	NIST Webbook
tf	371.00 ± 0.03	K	NIST Webbook
tf	371.00 ± 0.30	K	NIST Webbook
tf	371.00 ± 0.30	K	NIST Webbook
tf	371.00 ± 0.30	K	NIST Webbook
tf	371.60	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	370.70 ± 1.00	K	NIST Webbook
tf	372.25	K	Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or n-butanol Mixture
tf	371.00 ± 0.50	K	NIST Webbook
tf	370.05 ± 0.50	K	NIST Webbook
tf	370.25	K	Aqueous Solubility Prediction Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.97	J/mol×K	780.63	Joback Method
cpg	238.55	J/mol×K	635.02	Joback Method
cpg	244.40	J/mol×K	664.14	Joback Method
cpg	249.96	J/mol×K	693.27	Joback Method
cpg	255.24	J/mol×K	722.39	Joback Method

cpg	260.24	J/mol×K	751.51	Joback Method
cpg	232.39	J/mol×K	605.90	Joback Method
dvisc	0.0000823	Pa×s	566.18	Joback Method
dvisc	0.0001541	Pa×s	526.47	Joback Method
dvisc	0.0003200	Pa×s	486.75	Joback Method
dvisc	0.0007563	Pa×s	447.04	Joback Method
dvisc	0.0021139	Pa×s	407.32	Joback Method
dvisc	0.0073782	Pa×s	367.61	Joback Method
dvisc	0.0000477	Pa×s	605.90	Joback Method
hfust	20.90	kJ/mol	371.00	NIST Webbook
hfust	20.70	kJ/mol	370.90	NIST Webbook
hfust	18.80	kJ/mol	363.90	NIST Webbook
hfust	21.30	kJ/mol	372.30	NIST Webbook
hfust	23.00	kJ/mol	371.00	NIST Webbook
hsubt	117.00 ± 1.20	kJ/mol	355.50	NIST Webbook
hsubt	132.30	kJ/mol	284.50	NIST Webbook
hsubt	134.00 ± 4.00	kJ/mol	331.00	NIST Webbook
hvapt	98.10	kJ/mol	502.00	NIST Webbook
pvap	0.17	kPa	433.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	0.32	kPa	443.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	0.55	kPa	453.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	473.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.86943e+01
Coeff. B	-6.35351e+03
Coeff. C	-1.24671e+02
Temperature range (K), min.	469.85
Temperature range (K), max.	599.42

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.83091e+02
Coeff. B	-2.04558e+04
Coeff. C	-2.28089e+01
Coeff. D	4.85058e-06
Temperature range (K), min.	370.65
Temperature range (K), max.	807.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
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 of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behavior of the bulk material for applications?:	https://www.doi.org/10.1016/j.tca.2014.09.022
Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, Succinic Acid, and Azelaic Acid in Cyclohexane + Cyclohexanol + Cyclohexanone Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.6b00800
Determination and Correlation for Solubility of Glutaric Acid in Cyclohexanone Mixtures:	https://www.doi.org/10.1021/acs.jced.6b00325
Odd–even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
Solubility of succinic acid, glutaric acid and adipic acid in propionic acid + epsilon-caprolactone + water mixtures:	https://www.doi.org/10.1016/j.jct.2019.06.033
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental measurement and thermodynamic modeling:	https://www.doi.org/10.1021/acs.jced.7b00468
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/je5003785
Solid–Liquid Equilibrium and Phase Diagram for the Ternary Succinic Acid + Glutaric Acid + Water System:	

Solid Liquid Equilibria for Six Binary Mixtures of Pentanedioic Acid, Octanedioic Acid, 3-Methylheptanedioic Acid, 2,2-Dimethylbutanedioic Acid, and 2,3-Dimethylbutanedioic Acid:	https://www.doi.org/10.1021/je400686f
Determination and correlation of solid-liquid phase equilibrium and phase diagram for multicomponent system of mixed dibasic acids. (III) Ternary system of succinic acid + glutaric acid + ethanol system:	https://www.doi.org/10.1016/j.jct.2016.12.010
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=964
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water:	https://www.doi.org/10.1021/je700027n
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility Determination and Thermodynamic Modeling of Glutaric Anhydride in Diverse Solvent Systems Consisting of Acetic Acid, Ethanoic Anhydride, and Tetrachloromethane from T = (278.15 to 324.45) K:	https://www.doi.org/10.1021/acs.jced.8b00496
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=964
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110941&Units=SI
Solubilities of Adipic Acid and Succinic Acid in Glutaric Acid + Acetone or n-Butanol Mixture:	https://www.doi.org/10.1021/je500682v
Volumetric properties of aqueous solutions of glutaric acid:	https://www.doi.org/10.1016/j.jct.2006.12.015
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 + ethanol system:	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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and Correlation for Solubilities of Succinic Acid and Glutaric Acid in e-Caprolactone + Acetic Acid Mixtures and e-Caprolactone + Cyclohexanone Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00660

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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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