Octanedioic acid

Other names:	1,6-Dicarboxyhexane
	1,6-Hexanedicarboxylic acid
	1,8-Octanedioic acid
	Cork acid
	Hexamethylenedicarboxylic acid
	Octane-1,8-dioic acid
	Suberic acid
Inchi:	InChI=1S/C8H14O4/c9-7(10)5-3-1-2-4-6-8(11)12/h1-6H2,(H,9,10)(H,11,12)
InchiKey:	TYFQFVWCELRYAO-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	O=C(O)CCCCCCC(=O)O
Mol. weight [g/mol]:	174.19
CAS:	505-48-6

Physical Properties

Property code	Value	Unit	Source
chs	-4110.90 ± 1.30	kJ/mol	NIST Webbook
gf	-515.00	kJ/mol	Joback Method
hf	-738.07	kJ/mol	Joback Method
hfus	2.00	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hfus	30.52	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
hsub	147.80 ± 3.80	kJ/mol	NIST Webbook
hsub	143.00 ± 4.00	kJ/mol	NIST Webbook
hvap	116.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.96		Aqueous Solubility Prediction Method
logp	1.496		Crippen Method
mcvol	138.460	ml/mol	McGowan Method

pc	2970.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	674.54	K	Joback Method
tc	847.61	K	Joback Method
tf	417.00 ± 1.50	K	NIST Webbook
tf	410.00 ± 3.00	K	NIST Webbook
tf	413.00 ± 4.00	K	NIST Webbook
tf	415.50 ± 0.50	K	NIST Webbook
tf	415.50 ± 0.40	K	NIST Webbook
tf	416.65	K	Aqueous Solubility Prediction Method
tf	415.50 ± 0.30	K	NIST Webbook
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.64	J/mol×K	674.54	Joback Method
cpg	381.25	J/mol×K	703.39	Joback Method
cpg	389.43	J/mol×K	732.23	Joback Method
cpg	397.21	J/mol×K	761.08	Joback Method
cpg	404.58	J/mol×K	789.92	Joback Method
cpg	411.58	J/mol×K	818.77	Joback Method
cpg	418.19	J/mol×K	847.61	Joback Method
dvisc	0.0000238	Pa×s	674.54	Joback Method
dvisc	0.0010352	Pa×s	446.94	Joback Method
dvisc	0.0003684	Pa×s	492.46	Joback Method
dvisc	0.0036765	Pa×s	401.42	Joback Method
dvisc	0.0000757	Pa×s	583.50	Joback Method
dvisc	0.0000407	Pa×s	629.02	Joback Method
dvisc	0.0001562	Pa×s	537.98	Joback Method
hfust	30.70	kJ/mol	413.20	NIST Webbook
hfust	28.82	kJ/mol	415.30	NIST Webbook
hfust	28.82	kJ/mol	415.30	NIST Webbook
hsubt	168.00 ± 7.00	kJ/mol	363.00	NIST Webbook
hsubt	148.00	kJ/mol	315.00	NIST Webbook
hsubt	143.10 ± 3.80	kJ/mol	393.00	NIST Webbook
hvapt	91.40	kJ/mol	532.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77470e+01
Coeff. B	-6.61200e+03
Coeff. C	-1.14691e+02
Temperature range (K), min.	493.40
Temperature range (K), max.	646.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.35392e+03
Coeff. B	-8.05167e+04
Coeff. C	-1.96409e+02
Coeff. D	1.13237e-04
Temperature range (K), min.	379.15
Temperature range (K), max.	619.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C505486&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=970

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=970

An odd-even effect on solubility of dicarboxylic acids in organic solvents: https://www.doi.org/10.1016/j.jct.2014.05.009

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Determination of the solubility, dissolution enthalpy and entropy of suberic acid in different solvents: https://www.doi.org/10.1016/j.fluid.2012.06.012

Solid Liquid Equilibria for Six Binary Mixtures of Pentanedioic Acid, Octanedioic Acid, 3-Methylpentanedioic Acid, 2,2-Dimethylbutanedioic Acid, and 2,3-Dimethylbutanedioic Acid:	https://www.doi.org/10.1021/je400686f
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids:	https://www.doi.org/10.1021/je0498356
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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