Hexadecanedioic acid

Other names:	.alpha.,.omega.-tetradecanedicarboxylic acid
	1,14-Tetradecanedicarboxylic acid
	1,16-Hexadecanedioic acid
	Hexadecane-1,16-dioic acid
	Thapsic acid
	n-Tetradecane-«omega»,«omega»'-dicarboxylic acid
	n-Tetradecane-Â«omegaÂ»,Â«omegaÂ»'-dicarboxylic acid
Inchi:	InChI=1S/C16H30O4/c17-15(18)13-11-9-7-5-3-1-2-4-6-8-10-12-14-16(19)20/h1-14H2,(H
InchiKey:	QQHJDPROMQRDLA-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	O=C(O)CCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	286.41
CAS:	505-54-4

Physical Properties

Property code	Value	Unit	Source
gf	-447.64	kJ/mol	Joback Method
hf	-903.19	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	151.00 ± 3.00	kJ/mol	NIST Webbook
hsub	155.40 ± 3.30	kJ/mol	NIST Webbook
hvap	98.06	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.617		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
tb	857.58	K	Joback Method
tc	1049.97	K	Joback Method
tf	491.58	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.11	J/mol×K	1017.90	Joback Method
cpg	855.31	J/mol×K	985.84	Joback Method
cpg	843.82	J/mol×K	953.77	Joback Method
cpg	831.61	J/mol×K	921.71	Joback Method
cpg	818.63	J/mol×K	889.64	Joback Method
cpg	804.86	J/mol×K	857.58	Joback Method
cpg	876.26	J/mol×K	1049.97	Joback Method
dvisc	0.0005811	Pa×s	491.58	Joback Method
dvisc	0.0000040	Pa×s	857.58	Joback Method
dvisc	0.0000066	Pa×s	796.58	Joback Method
dvisc	0.0000120	Pa×s	735.58	Joback Method
dvisc	0.0000244	Pa×s	674.58	Joback Method
dvisc	0.0000568	Pa×s	613.58	Joback Method
dvisc	0.0001598	Pa×s	552.58	Joback Method
hfust	52.20	kJ/mol	395.40	NIST Webbook
hsubt	151.00 ± 3.30	kJ/mol	387.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42133e+01
Coeff. B	-5.69422e+03
Coeff. C	-1.30771e+02
Temperature range (K), min.	539.67
Temperature range (K), max.	770.44

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C505544&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume