1,16-Hexadecanediol

Other names:	1,16-dihydroxyhexadecane
	hexadecane-1,16-diol
Inchi:	InChI=1S/C16H34O2/c17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-18/h17-18H,1-16H2
InchiKey:	GJBXIPOYHVMPQJ-UHFFFAOYSA-N
Formula:	C16H34O2
SMILES:	OCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	258.44
CAS:	7735-42-4

Physical Properties

Property code	Value	Unit	Source
gf	-189.80	kJ/mol	Joback Method
hf	-678.03	kJ/mol	Joback Method
hfus	45.37	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.432		Crippen Method
mcvol	248.040	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	749.84	K	Joback Method
tc	919.16	K	Joback Method
tf	366.00	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.14	J/mol×K	749.84	Joback Method

cpg	781.76	J/mol×K	778.06	Joback Method
cpg	796.67	J/mol×K	806.28	Joback Method
cpg	810.91	J/mol×K	834.50	Joback Method
cpg	824.49	J/mol×K	862.72	Joback Method
cpg	837.45	J/mol×K	890.94	Joback Method
cpg	849.80	J/mol×K	919.16	Joback Method
dvisc	0.0006747	Pa×s	451.41	Joback Method
dvisc	0.0039775	Pa×s	391.72	Joback Method
dvisc	0.0001732	Pa×s	511.09	Joback Method
dvisc	0.0000591	Pa×s	570.78	Joback Method
dvisc	0.0000247	Pa×s	630.47	Joback Method
dvisc	0.0000120	Pa×s	690.15	Joback Method
dvisc	0.0000066	Pa×s	749.84	Joback Method
hfust	64.20	kJ/mol	365.40	NIST Webbook
hvapt	163.30	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.68254e+01
Coeff. B	-1.02416e+04
Coeff. C	-1.22262e+02
Temperature range (K), min.	508.19
Temperature range (K), max.	598.31

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7735424&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect:	https://www.doi.org/10.1016/j.jct.2013.08.019

Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography: https://www.doi.org/10.1021/je060333x

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume