Hexadecane-1,2-diol

Other names: 1,2-Hexadecanediol
hexadecane-1,16-diol
Inchi: InChI=1S/C16H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16(18)15-17/h16-18H,2-15H2,1
InchiKey: BTOOAFQCTJZDRC-UHFFFAOYSA-N
Formula: C16H34O2
SMILES: CCCCCCCCCCCCCCC(O)CO
Mol. weight [g/mol]: 258.44
CAS: 6920-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-192.24	kJ/mol	Joback Method
hf	-683.31	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.431		Crippen Method
mcvol	248.040	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2031.00		NIST Webbook
tb	749.40	K	Joback Method
tc	919.21	K	Joback Method
tf	348.65 ± 0.50	K	NIST Webbook
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.64	J/mol×K	749.40	Joback Method
cpg	782.32	J/mol×K	777.70	Joback Method
cpg	797.28	J/mol×K	806.00	Joback Method
cpg	811.55	J/mol×K	834.30	Joback Method
cpg	825.16	J/mol×K	862.60	Joback Method
cpg	838.13	J/mol×K	890.90	Joback Method

cpg	850.49	J/mol×K	919.21	Joback Method
dvisc	0.0065622	Pa×s	376.72	Joback Method
dvisc	0.0008978	Pa×s	438.83	Joback Method
dvisc	0.0002012	Pa×s	500.95	Joback Method
dvisc	0.0000627	Pa×s	563.06	Joback Method
dvisc	0.0000246	Pa×s	625.17	Joback Method
dvisc	0.0000115	Pa×s	687.29	Joback Method
dvisc	0.0000061	Pa×s	749.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.35157e+01
Coeff. B	-8.79049e+03
Coeff. C	-1.18278e+02
Temperature range (K), min.	496.72
Temperature range (K), max.	601.16

Sources

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=C6920247&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

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