4-Hexadecanol

Inchi: InChI=1S/C16H34O/c1-3-5-6-7-8-9-10-11-12-13-15-16(17)14-4-2/h16-17H,3-15H2,1-2H3
InchiKey: JIMMILCKVYOFET-UHFFFAOYSA-N
Formula: C16H34O
SMILES: CCCCCCCCCCCCC(O)CCC
Mol. weight [g/mol]: 242.44
CAS: 19781-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-55.42	kJ/mol	Joback Method
hf	-531.08	kJ/mol	Joback Method
hfus	37.76	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.458		Crippen Method
mcvol	242.170	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
tb	657.22	K	Joback Method
tc	818.60	K	Joback Method
tf	315.90	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.99	J/mol×K	657.22	Joback Method
cpg	710.14	J/mol×K	684.12	Joback Method
cpg	726.57	J/mol×K	711.01	Joback Method
cpg	742.31	J/mol×K	737.91	Joback Method
cpg	757.38	J/mol×K	764.81	Joback Method
cpg	771.81	J/mol×K	791.70	Joback Method
cpg	785.60	J/mol×K	818.60	Joback Method
dvisc	0.0136883	Pa×s	315.90	Joback Method
dvisc	0.0024349	Pa×s	372.79	Joback Method

dvisc	0.0006842	Pa×s	429.67	Joback Method
dvisc	0.0002587	Pa×s	486.56	Joback Method
dvisc	0.0001199	Pa×s	543.45	Joback Method
dvisc	0.0000643	Pa×s	600.33	Joback Method
dvisc	0.0000384	Pa×s	657.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54102e+01
Coeff. B	-5.25255e+03
Coeff. C	-1.01709e+02
Temperature range (K), min.	449.04
Temperature range (K), max.	621.83

Sources

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
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=C19781432&Units=SI

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