2-Hexadecanol

Other names: Hexadecanol-2
hexadecan-2-ol
Inchi: InChI=1S/C16H34O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16(2)17/h16-17H,3-15H2,1-2H3
InchiKey: FVDRFBGMOWJEOR-UHFFFAOYSA-N
Formula: C16H34O
SMILES: CCCCCCCCCCCCCCC(C)O
Mol. weight [g/mol]: 242.44
CAS: 14852-31-4

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
rinpol	1702.00		NIST Webbook
rinpol	1702.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2312.00		NIST Webbook
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
hvapt	102.20	kJ/mol	393.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62043e+01
Coeff. B	-5.60812e+03
Coeff. C	-1.04378e+02
Temperature range (K), min.	456.72
Temperature range (K), max.	619.22

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14852314&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

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