

5-Hexadecanol

Other names:	hexadecan-5-ol
Inchi:	InChI=1S/C16H34O/c1-3-5-7-8-9-10-11-12-13-15-16(17)14-6-4-2/h16-17H,3-15H2,1-2H3
InchiKey:	HNDLTSNUZCYNRL-UHFFFAOYSA-N
Formula:	C16H34O
SMILES:	CCCCCCCCCCCC(O)CCCC
Mol. weight [g/mol]:	242.44
CAS:	21078-87-5

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/molxK	657.22	Joback Method
cpg	710.14	J/molxK	684.12	Joback Method
cpg	726.57	J/molxK	711.01	Joback Method
cpg	742.31	J/molxK	737.91	Joback Method
cpg	757.38	J/molxK	764.81	Joback Method
cpg	771.81	J/molxK	791.70	Joback Method
cpg	785.60	J/molxK	818.60	Joback Method
dvisc	0.0136883	Paxs	315.90	Joback Method

dvisc	0.0024349	Paxs	372.79	Joback Method
dvisc	0.0006842	Paxs	429.67	Joback Method
dvisc	0.0002587	Paxs	486.56	Joback Method
dvisc	0.0001199	Paxs	543.45	Joback Method
dvisc	0.0000643	Paxs	600.33	Joback Method
dvisc	0.0000384	Paxs	657.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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=C21078875&Units=SI

Legend

cp_g:	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

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