1-Hexadecanol, acetate

Other names:	1-Acetoxyhexadecane
	1-Hexadecanol, 1-acetate
	Acelan A
	Acetic acid, hexadecyl ester
	Acrylated lanolin alcohol
	Cetyl acetate
	ENT 1025
	Hexadecanyl acetate
	Hexadecyl acetate
	NSC 8492
	Palmityl acetate
	n-Hexadecyl acetate
	n-Hexadecyl ethanoate
Inchi:	InChI=1S/C18H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h3-17H2,1-2
InchiKey:	LSTDYDRCKUBPDI-UHFFFAOYSA-N
Formula:	C18H36O2
SMILES:	CCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	284.48
CAS:	629-70-9

Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-659.65	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	102.30	kJ/mol	NIST Webbook
log10ws	-6.22		Crippen Method
logp	6.031		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	1994.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1991.10		NIST Webbook

rinpol	1984.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2006.90		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	2006.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	2009.00		NIST Webbook
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rinpol	2010.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2008.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2309.00		NIST Webbook
tb	687.53	K	Joback Method
tc	855.83	K	Joback Method
tf	292.35 ± 2.00	K	NIST Webbook
tf	295.40 ± 1.50	K	NIST Webbook
tf	291.70 ± 4.00	K	NIST Webbook
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.54	J/mol×K	855.83	Joback Method
cpg	789.92	J/mol×K	687.53	Joback Method
cpg	808.70	J/mol×K	715.58	Joback Method
cpg	826.65	J/mol×K	743.63	Joback Method
cpg	843.80	J/mol×K	771.68	Joback Method
cpg	860.14	J/mol×K	799.73	Joback Method
cpg	875.72	J/mol×K	827.78	Joback Method
dvisc	0.0000953	Pa×s	687.53	Joback Method
dvisc	0.0020226	Pa×s	364.78	Joback Method
dvisc	0.0008765	Pa×s	418.57	Joback Method
dvisc	0.0004595	Pa×s	472.36	Joback Method
dvisc	0.0002749	Pa×s	526.15	Joback Method
dvisc	0.0001809	Pa×s	579.95	Joback Method
dvisc	0.0001278	Pa×s	633.74	Joback Method
hvapt	70.30	kJ/mol	450.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24900e+01
Coeff. B	-8.50187e+03
Coeff. C	-1.24394e+02
Temperature range (K), min.	507.32
Temperature range (K), max.	619.31

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1134.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629709&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
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