tetradecyl acetate

Other names:	1-tetradecanol, acetate
	1-tetradecyl acetate
	acetic acid, tetradecyl ester
	myristyl acetate
	tetradecyl ethanoate
Inchi:	InChI=1S/C16H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h3-15H2,1-2H3
InchiKey:	IOUUIFSIQMVYKP-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	256.42
CAS:	638-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	89.90 ± 0.20	kJ/mol	NIST Webbook
hvap	91.70	kJ/mol	NIST Webbook
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1806.20		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1793.00		NIST Webbook
rinpol	1811.00		NIST Webbook

rinpol	1780.00		NIST Webbook
rinpol	1790.60		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1793.00		NIST Webbook
rinpol	1806.20		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1790.60		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	287.15 ± 0.20	K	NIST Webbook
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method
hvapt	72.70	kJ/mol	436.50	NIST Webbook

pvap	2.40e-04	kPa	319.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.05e-03	kPa	334.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	7.80e-04	kPa	331.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.00e-04	kPa	328.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.50e-04	kPa	325.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.30e-04	kPa	322.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.40e-03	kPa	337.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.80e-04	kPa	316.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.30e-04	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	9.00e-05	kPa	310.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.00e-05	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.00e-05	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.86e-03	kPa	340.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.00994e+01
Coeff. B	-7.13143e+03
Coeff. C	-1.12162e+02
Temperature range (K), min.	472.12
Temperature range (K), max.	594.41

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates:	https://www.doi.org/10.1016/j.jct.2005.08.003
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=C638595&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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