1-Pentadecanol acetate

Other names: Acetic acid, pentadecyl ester
Pentadecyl acetate
n-Pentadecyl acetate
Inchi: InChI=1S/C17H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-17(2)18/h3-16H2,1-2H3
InchiKey: AAAIZLQILBFRTJ-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 270.45
CAS: 629-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-141.66	kJ/mol	Joback Method
hf	-639.01	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.641		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1907.40		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	664.65	K	Joback Method
tc	832.26	K	Joback Method
tf	353.51	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.28	J/mol×K	664.65	Joback Method
cpg	750.62	J/mol×K	692.59	Joback Method

cpg	768.17	J/mol×K	720.52	Joback Method
cpg	784.95	J/mol×K	748.46	Joback Method
cpg	800.97	J/mol×K	776.39	Joback Method
cpg	816.25	J/mol×K	804.33	Joback Method
cpg	830.80	J/mol×K	832.26	Joback Method
dvisc	0.0022120	Pa×s	353.51	Joback Method
dvisc	0.0009695	Pa×s	405.37	Joback Method
dvisc	0.0005124	Pa×s	457.22	Joback Method
dvisc	0.0003083	Pa×s	509.08	Joback Method
dvisc	0.0002038	Pa×s	560.94	Joback Method
dvisc	0.0001445	Pa×s	612.79	Joback Method
dvisc	0.0001081	Pa×s	664.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.12034e+01
Coeff. B	-7.76900e+03
Coeff. C	-1.18278e+02
Temperature range (K), min.	489.72
Temperature range (K), max.	607.14

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=C629583&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume