1-Octadecanol, 5-chloro, acetate

Other names: 5-Chlorooctadecyl acetate
Inchi: InChI=1S/C20H39ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-16-20(21)17-14-15-18-23-19(2)22/
InchiKey: QNEYPSPGGCHRQB-UHFFFAOYSA-N
Formula: C20H39ClO2
SMILES: CCCCCCCCCCCCCC(Cl)CCCCOC(C)=O
Mol. weight [g/mol]: 346.98

Physical Properties

Property code	Value	Unit	Source
gf	-130.77	kJ/mol	Joback Method
hf	-721.95	kJ/mol	Joback Method
hfus	51.02	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	7.028		Crippen Method
mcvol	312.340	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2383.00		NIST Webbook
rinpol	2383.00		NIST Webbook
ripol	2892.00		NIST Webbook
ripol	2882.00		NIST Webbook
tb	770.28	K	Joback Method
tc	948.76	K	Joback Method
tf	402.24	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.69	J/mol×K	770.28	Joback Method
cpg	963.67	J/mol×K	800.03	Joback Method
cpg	981.68	J/mol×K	829.77	Joback Method
cpg	998.75	J/mol×K	859.52	Joback Method
cpg	1014.91	J/mol×K	889.27	Joback Method

cpg	1030.18	J/mol×K	919.02	Joback Method
cpg	1044.59	J/mol×K	948.76	Joback Method
dvisc	0.0015827	Pa×s	402.24	Joback Method
dvisc	0.0006361	Pa×s	463.58	Joback Method
dvisc	0.0003163	Pa×s	524.92	Joback Method
dvisc	0.0001821	Pa×s	586.26	Joback Method
dvisc	0.0001164	Pa×s	647.60	Joback Method
dvisc	0.0000804	Pa×s	708.94	Joback Method
dvisc	0.0000589	Pa×s	770.28	Joback Method

Sources

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=R33573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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