Octadecyl 2-chlorobutanoate

Other names: Butanoic acid, 2-chloro, octadecyl ester
Inchi: InChI=1S/C22H43ClO2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-22(24)21(2
InchiKey: IQOGLHRADJQOGE-UHFFFAOYSA-N
Formula: C22H43ClO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(Cl)CC
Mol. weight [g/mol]: 375.03

Physical Properties

Property code	Value	Unit	Source
gf	-113.93	kJ/mol	Joback Method
hf	-763.23	kJ/mol	Joback Method
hfus	56.20	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.809		Crippen Method
mcvol	340.520	ml/mol	McGowan Method
pc	911.08	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	816.04	K	Joback Method
tc	1000.35	K	Joback Method
tf	424.78	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.19	J/mol×K	816.04	Joback Method
cpg	1087.04	J/mol×K	846.76	Joback Method
cpg	1105.82	J/mol×K	877.48	Joback Method
cpg	1123.55	J/mol×K	908.19	Joback Method
cpg	1140.27	J/mol×K	938.91	Joback Method
cpg	1156.02	J/mol×K	969.63	Joback Method

cpg	1170.82	J/mol×K	1000.35	Joback Method
dvisc	0.0012419	Pa×s	424.78	Joback Method
dvisc	0.0004914	Pa×s	489.99	Joback Method
dvisc	0.0002417	Pa×s	555.20	Joback Method
dvisc	0.0001380	Pa×s	620.41	Joback Method
dvisc	0.0000877	Pa×s	685.62	Joback Method
dvisc	0.0000603	Pa×s	750.83	Joback Method
dvisc	0.0000440	Pa×s	816.04	Joback Method

Sources

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=R28326&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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