Tetradecyl 4-chlorobutanoate

Other names: Butanoic acid, 4-chloro, tetradecyl ester
Inchi: InChI=1S/C18H35ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-21-18(20)15-14-16-19/h2-17H
InchiKey: WSGHRRURYBZEDT-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 318.92

Physical Properties

Property code	Value	Unit	Source
gf	-145.17	kJ/mol	Joback Method
hf	-675.39	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.250		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2211.00		NIST Webbook
tb	724.96	K	Joback Method
tc	898.71	K	Joback Method
tf	394.70	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.31	J/mol×K	724.96	Joback Method
cpg	843.30	J/mol×K	753.92	Joback Method
cpg	860.43	J/mol×K	782.88	Joback Method
cpg	876.73	J/mol×K	811.84	Joback Method
cpg	892.21	J/mol×K	840.79	Joback Method
cpg	906.90	J/mol×K	869.75	Joback Method
cpg	920.82	J/mol×K	898.71	Joback Method
dvisc	0.0015927	Pa×s	394.70	Joback Method

dvisc	0.0007235	Pa×s	449.74	Joback Method
dvisc	0.0003904	Pa×s	504.79	Joback Method
dvisc	0.0002378	Pa×s	559.83	Joback Method
dvisc	0.0001583	Pa×s	614.87	Joback Method
dvisc	0.0001127	Pa×s	669.92	Joback Method
dvisc	0.0000844	Pa×s	724.96	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=R28479&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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