3-Chloropropionic acid, tetradecyl ester

Other names: Propanoic acid, 3-chloro, tetradecyl ester
Tetradecyl 3-chloropropanoate
Inchi: InChI=1S/C17H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-20-17(19)14-15-18/h2-16H2,
InchiKey: KUZUNHDCZIJWAO-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCl
Mol. weight [g/mol]: 304.90
CAS: 64120-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-153.59	kJ/mol	Joback Method
hf	-654.75	kJ/mol	Joback Method
hfus	46.77	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.860		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2110.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2572.00		NIST Webbook
ripol	2587.00		NIST Webbook
ripol	2602.00		NIST Webbook
ripol	2572.00		NIST Webbook
tb	702.08	K	Joback Method
tc	874.86	K	Joback Method
tf	383.43	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.38	J/mol×K	702.08	Joback Method
cpg	784.94	J/mol×K	730.88	Joback Method
cpg	801.69	J/mol×K	759.67	Joback Method
cpg	817.63	J/mol×K	788.47	Joback Method
cpg	832.80	J/mol×K	817.27	Joback Method
cpg	847.21	J/mol×K	846.07	Joback Method
cpg	860.88	J/mol×K	874.86	Joback Method
dvisc	0.0017567	Pa×s	383.43	Joback Method
dvisc	0.0008072	Pa×s	436.54	Joback Method
dvisc	0.0004391	Pa×s	489.65	Joback Method
dvisc	0.0002691	Pa×s	542.75	Joback Method
dvisc	0.0001799	Pa×s	595.86	Joback Method
dvisc	0.0001285	Pa×s	648.97	Joback Method
dvisc	0.0000966	Pa×s	702.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64120167&Units=SI
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

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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