Propanoic acid, 2-chloro, tetradecyl ester

Other names: Tetradecyl 2-chloropropanoate
Inchi: InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-17(19)16(2)18/h16H,3-15
InchiKey: FVMWGIBSMXRINW-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 304.90

Physical Properties

Property code	Value	Unit	Source
gf	-156.03	kJ/mol	Joback Method
hf	-660.03	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.858		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2036.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2039.00		NIST Webbook
ripol	2450.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2414.00		NIST Webbook
ripol	2436.00		NIST Webbook
ripol	2427.00		NIST Webbook
tb	701.64	K	Joback Method
tc	876.28	K	Joback Method
tf	368.43	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.83	J/mol×K	701.64	Joback Method
cpg	785.61	J/mol×K	730.75	Joback Method
cpg	802.54	J/mol×K	759.85	Joback Method
cpg	818.65	J/mol×K	788.96	Joback Method
cpg	833.96	J/mol×K	818.07	Joback Method
cpg	848.48	J/mol×K	847.17	Joback Method
cpg	862.24	J/mol×K	876.28	Joback Method
dvisc	0.0022085	Pa×s	368.43	Joback Method
dvisc	0.0009117	Pa×s	423.97	Joback Method
dvisc	0.0004619	Pa×s	479.50	Joback Method
dvisc	0.0002695	Pa×s	535.03	Joback Method
dvisc	0.0001741	Pa×s	590.57	Joback Method
dvisc	0.0001212	Pa×s	646.11	Joback Method
dvisc	0.0000893	Pa×s	701.64	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=R23607&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