Undecyl 4-chlorobutanoate

Other names: Butanoic acid, 4-chloro, undecyl ester
Inchi: InChI=1S/C15H29ClO2/c1-2-3-4-5-6-7-8-9-10-14-18-15(17)12-11-13-16/h2-14H2,1H3
InchiKey: KZEWKNYKRXBAPR-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: CCCCCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 276.84

Physical Properties

Property code	Value	Unit	Source
gf	-170.43	kJ/mol	Joback Method
hf	-613.47	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.079		Crippen Method
mcvol	241.890	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	656.32	K	Joback Method
tc	828.65	K	Joback Method
tf	360.89	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.00	J/mol×K	656.32	Joback Method
cpg	671.67	J/mol×K	685.04	Joback Method
cpg	687.59	J/mol×K	713.76	Joback Method

cpg	702.78	J/mol×K	742.49	Joback Method
cpg	717.25	J/mol×K	771.21	Joback Method
cpg	731.03	J/mol×K	799.93	Joback Method
cpg	744.13	J/mol×K	828.65	Joback Method
dvisc	0.0021007	Pa×s	360.89	Joback Method
dvisc	0.0009897	Pa×s	410.13	Joback Method
dvisc	0.0005479	Pa×s	459.37	Joback Method
dvisc	0.0003401	Pa×s	508.60	Joback Method
dvisc	0.0002297	Pa×s	557.84	Joback Method
dvisc	0.0001653	Pa×s	607.08	Joback Method
dvisc	0.0001250	Pa×s	656.32	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=R28504&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