Undecyl 3-chlorobutanoate

Other names: Butanoic acid, 3-chloro, undecyl ester
Inchi: InChI=1S/C15H29ClO2/c1-3-4-5-6-7-8-9-10-11-12-18-15(17)13-14(2)16/h14H,3-13H2,1-
InchiKey: ANPLFFNNFIHAGT-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: CCCCCCCCCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 276.84

Physical Properties

Property code	Value	Unit	Source
gf	-172.87	kJ/mol	Joback Method
hf	-618.75	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	62.14	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	5.078		Crippen Method
mcvol	241.890	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	655.88	K	Joback Method
tc	830.56	K	Joback Method
tf	345.89	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.43	J/mol×K	655.88	Joback Method

cpg	732.49	J/mol×K	801.45	Joback Method
cpg	718.56	J/mol×K	772.34	Joback Method
cpg	703.90	J/mol×K	743.22	Joback Method
cpg	688.50	J/mol×K	714.11	Joback Method
cpg	672.35	J/mol×K	684.99	Joback Method
cpg	745.72	J/mol×K	830.56	Joback Method
dvisc	0.0001161	Pa×s	655.88	Joback Method
dvisc	0.0001566	Pa×s	604.21	Joback Method
dvisc	0.0002236	Pa×s	552.55	Joback Method
dvisc	0.0003436	Pa×s	500.88	Joback Method
dvisc	0.0005826	Pa×s	449.22	Joback Method
dvisc	0.0011334	Pa×s	397.56	Joback Method
dvisc	0.0026899	Pa×s	345.89	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28497&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume