3-Chlropropionic acid, undecyl ester

Other names: Propanoic acid, 3-chloro, undecyl ester
Inchi: InChI=1S/C14H27ClO2/c1-2-3-4-5-6-7-8-9-10-13-17-14(16)11-12-15/h2-13H2,1H3
InchiKey: MEBJHQDVCFHKMD-UHFFFAOYSA-N
Formula: C14H27ClO2
SMILES: CCCCCCCCCCCOC(=O)CCCl
Mol. weight [g/mol]: 262.82
CAS: 74306-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-178.85	kJ/mol	Joback Method
hf	-592.83	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.689		Crippen Method
mcvol	227.800	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1807.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2308.00		NIST Webbook
ripol	2297.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2274.00		NIST Webbook
tb	633.44	K	Joback Method
tc	806.19	K	Joback Method
tf	349.62	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.72	J/mol×K	633.44	Joback Method
cpg	674.62	J/mol×K	777.39	Joback Method
cpg	661.20	J/mol×K	748.60	Joback Method
cpg	647.12	J/mol×K	719.81	Joback Method
cpg	632.35	J/mol×K	691.02	Joback Method
cpg	616.89	J/mol×K	662.23	Joback Method
cpg	687.38	J/mol×K	806.19	Joback Method
dvisc	0.0001413	Pa×s	633.44	Joback Method
dvisc	0.0001863	Pa×s	586.14	Joback Method
dvisc	0.0002578	Pa×s	538.83	Joback Method
dvisc	0.0003797	Pa×s	491.53	Joback Method
dvisc	0.0006073	Pa×s	444.23	Joback Method
dvisc	0.0010865	Pa×s	396.92	Joback Method
dvisc	0.0022752	Pa×s	349.62	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=C74306073&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