Lauric acid «beta»-chloroethyl ester

Other names: 2-Chloroethyl laurate
2-Chloroethyl dodecanoate
Dodecanoic acid, 2-chloroethyl ester
Inchi: InChI=1S/C14H27ClO2/c1-2-3-4-5-6-7-8-9-10-11-14(16)17-13-12-15/h2-13H2,1H3
InchiKey: PPRUSMUBWUQYRY-UHFFFAOYSA-N
Formula: C14H27ClO2
SMILES: CCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 262.82
CAS: 64919-15-9

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	1800.00		NIST Webbook
rinpol	1793.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1792.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2301.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2268.00		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	616.89	J/mol×K	662.23	Joback Method
cpg	632.35	J/mol×K	691.02	Joback Method
cpg	647.12	J/mol×K	719.81	Joback Method
cpg	661.20	J/mol×K	748.60	Joback Method
cpg	674.62	J/mol×K	777.39	Joback Method
cpg	687.38	J/mol×K	806.19	Joback Method
dvisc	0.0022752	Pa×s	349.62	Joback Method
dvisc	0.0010865	Pa×s	396.92	Joback Method
dvisc	0.0006073	Pa×s	444.23	Joback Method
dvisc	0.0003797	Pa×s	491.53	Joback Method
dvisc	0.0002578	Pa×s	538.83	Joback Method
dvisc	0.0001863	Pa×s	586.14	Joback Method
dvisc	0.0001413	Pa×s	633.44	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=C64919159&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume