5-Chlorotetradecanoic acid, methyl ester

Inchi: InChI=1S/C15H29ClO2/c1-3-4-5-6-7-8-9-11-14(16)12-10-13-15(17)18-2/h14H,3-13H2,1-
InchiKey: MEUOMZCBLTYSNN-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: CCCCCCCCCC(Cl)CCCC(=O)OC
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	1892.00		NIST Webbook
ripol	2339.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R309576&Units=SI

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