14-Chlorotetradecanoic acid, methyl ester

Inchi: InChI=1S/C15H29ClO2/c1-18-15(17)13-11-9-7-5-3-2-4-6-8-10-12-14-16/h2-14H2,1H3
InchiKey: CZWCOVYSFRIKQU-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: COC(=O)CCCCCCCCCCCCCCCl
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	1981.00		NIST Webbook
rinpol	1981.00		NIST Webbook
ripol	2486.00		NIST Webbook
ripol	2486.00		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	731.03	J/mol×K	799.93	Joback Method
cpg	717.25	J/mol×K	771.21	Joback Method
cpg	702.78	J/mol×K	742.49	Joback Method
cpg	687.59	J/mol×K	713.76	Joback Method
cpg	671.67	J/mol×K	685.04	Joback Method

cpg	744.13	J/mol×K	828.65	Joback Method
dvisc	0.0001250	Pa×s	656.32	Joback Method
dvisc	0.0001653	Pa×s	607.08	Joback Method
dvisc	0.0002297	Pa×s	557.84	Joback Method
dvisc	0.0003401	Pa×s	508.60	Joback Method
dvisc	0.0005479	Pa×s	459.37	Joback Method
dvisc	0.0009897	Pa×s	410.13	Joback Method
dvisc	0.0021007	Pa×s	360.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R309036&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

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