3-Chlorotetradecanoic acid, methyl ester

Inchi: InChI=1S/C15H29ClO2/c1-3-4-5-6-7-8-9-10-11-12-14(16)13-15(17)18-2/h14H,3-13H2,1-
InchiKey: MKOKIXHEIXCUAP-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: CCCCCCCCCCCC(Cl)CC(=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	1863.00		NIST Webbook
rinpol	1863.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2279.00		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	672.35	J/mol×K	684.99	Joback Method
cpg	688.50	J/mol×K	714.11	Joback Method
cpg	703.90	J/mol×K	743.22	Joback Method
cpg	718.56	J/mol×K	772.34	Joback Method
cpg	732.49	J/mol×K	801.45	Joback Method

cpg	745.72	J/mol×K	830.56	Joback Method
dvisc	0.0026899	Pa×s	345.89	Joback Method
dvisc	0.0011334	Pa×s	397.56	Joback Method
dvisc	0.0005826	Pa×s	449.22	Joback Method
dvisc	0.0003436	Pa×s	500.88	Joback Method
dvisc	0.0002236	Pa×s	552.55	Joback Method
dvisc	0.0001566	Pa×s	604.21	Joback Method
dvisc	0.0001161	Pa×s	655.88	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=R309318&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