

13-Chlorotetradecanoic acid, methyl ester

Inchi:	InChI=1S/C15H29ClO2/c1-14(16)12-10-8-6-4-3-5-7-9-11-13-15(17)18-2/h14H,3-13H2,1-
InchiKey:	SUTDGNBOEWIVQM-UHFFFAOYSA-N
Formula:	C15H29ClO2
SMILES:	COC(=O)CCCCCCCCCCCC(C)Cl
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
ripol	1929.00		NIST Webbook
ripol	1929.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2406.00		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/molxK	655.88	Joback Method
cpg	672.35	J/molxK	684.99	Joback Method
cpg	688.50	J/molxK	714.11	Joback Method
cpg	703.90	J/molxK	743.22	Joback Method
cpg	718.56	J/molxK	772.34	Joback Method
cpg	732.49	J/molxK	801.45	Joback Method

cpg	745.72	J/molxK	830.56	Joback Method
dvisc	0.0026899	Paxs	345.89	Joback Method
dvisc	0.0011334	Paxs	397.56	Joback Method
dvisc	0.0005826	Paxs	449.22	Joback Method
dvisc	0.0003436	Paxs	500.88	Joback Method
dvisc	0.0002236	Paxs	552.55	Joback Method
dvisc	0.0001566	Paxs	604.21	Joback Method
dvisc	0.0001161	Paxs	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=R308979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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