

11-Chlorotridecanoic acid, methyl ester

Inchi:	InChI=1S/C14H27ClO2/c1-3-13(15)11-9-7-5-4-6-8-10-12-14(16)17-2/h13H,3-12H2,1-2H3
InchiKey:	UJZQWPACLYXMFK-UHFFFAOYSA-N
Formula:	C14H27ClO2
SMILES:	CCC(Cl)CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	262.82

Physical Properties

Property code	Value	Unit	Source
gf	-181.29	kJ/mol	Joback Method
hf	-598.11	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.688		Crippen Method
mcvol	227.800	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
ripol	1817.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2249.00		NIST Webbook
tb	633.00	K	Joback Method
tc	808.33	K	Joback Method
tf	334.62	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.12	J/molxK	633.00	Joback Method
cpg	617.58	J/molxK	662.22	Joback Method
cpg	633.29	J/molxK	691.44	Joback Method
cpg	648.28	J/molxK	720.66	Joback Method
cpg	662.56	J/molxK	749.89	Joback Method
cpg	676.15	J/molxK	779.11	Joback Method
cpg	689.06	J/molxK	808.33	Joback Method

dvisc	0.0029420	Paxs	334.62	Joback Method
dvisc	0.0012536	Paxs	384.35	Joback Method
dvisc	0.0006495	Paxs	434.08	Joback Method
dvisc	0.0003852	Paxs	483.81	Joback Method
dvisc	0.0002518	Paxs	533.54	Joback Method
dvisc	0.0001770	Paxs	583.27	Joback Method
dvisc	0.0001315	Paxs	633.00	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=R308855&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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