9-Chlorotridecanoic acid, methyl ester

Inchi: InChI=1S/C14H27ClO2/c1-3-4-10-13(15)11-8-6-5-7-9-12-14(16)17-2/h13H,3-12H2,1-2H3
InchiKey: NYHZZSFURRIPRD-UHFFFAOYSA-N
Formula: C14H27ClO2
SMILES: CCCCC(Cl)CCCCCCCC(=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
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2222.00		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/mol×K	633.00	Joback Method
cpg	676.15	J/mol×K	779.11	Joback Method
cpg	662.56	J/mol×K	749.89	Joback Method
cpg	648.28	J/mol×K	720.66	Joback Method
cpg	633.29	J/mol×K	691.44	Joback Method
cpg	617.58	J/mol×K	662.22	Joback Method

cpg	689.06	J/mol×K	808.33	Joback Method
dvisc	0.0001315	Pa×s	633.00	Joback Method
dvisc	0.0001770	Pa×s	583.27	Joback Method
dvisc	0.0002518	Pa×s	533.54	Joback Method
dvisc	0.0003852	Pa×s	483.81	Joback Method
dvisc	0.0006495	Pa×s	434.08	Joback Method
dvisc	0.0012536	Pa×s	384.35	Joback Method
dvisc	0.0029420	Pa×s	334.62	Joback Method

Sources

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=R310011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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