

# 3-Chlorotridecanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C14H27ClO2/c1-3-4-5-6-7-8-9-10-11-13(15)12-14(16)17-2/h13H,3-12H2,1-2H3
<b>InchiKey:</b>	ASQNHNBVEAFONI-UHFFFAOYSA-N
<b>Formula:</b>	C14H27ClO2
<b>SMILES:</b>	CCCCCCCCCCC(Cl)CC(=O)OC
<b>Mol. weight [g/mol]:</b>	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	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2142.00		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/mol×K	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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R309323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R309323&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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