

# 13-Chlorotridecanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C14H27ClO2/c1-17-14(16)12-10-8-6-4-2-3-5-7-9-11-13-15/h2-13H2,1H3
<b>InchiKey:</b>	KABAILADUUZJOR-UHFFFAOYSA-N
<b>Formula:</b>	C14H27ClO2
<b>SMILES:</b>	COC(=O)CCCCCCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	262.82

## Physical Properties

Property code	Value	Unit	Source
gf	-178.85	kJ/mol	Joback Method
hf	-592.83	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.689		Crippen Method
mcvol	227.800	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2330.00		NIST Webbook
tb	633.44	K	Joback Method
tc	806.19	K	Joback Method
tf	349.62	K	Joback Method
vc	0.892	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.72	J/molxK	633.44	Joback Method
cpg	616.89	J/molxK	662.23	Joback Method
cpg	632.35	J/molxK	691.02	Joback Method
cpg	647.12	J/molxK	719.81	Joback Method
cpg	661.20	J/molxK	748.60	Joback Method
cpg	674.62	J/molxK	777.39	Joback Method

cpg	687.38	J/molxK	806.19	Joback Method
dvisc	0.0022752	Paxs	349.62	Joback Method
dvisc	0.0010865	Paxs	396.92	Joback Method
dvisc	0.0006073	Paxs	444.23	Joback Method
dvisc	0.0003797	Paxs	491.53	Joback Method
dvisc	0.0002578	Paxs	538.83	Joback Method
dvisc	0.0001863	Paxs	586.14	Joback Method
dvisc	0.0001413	Paxs	633.44	Joback Method

## Sources

<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>
<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=R308984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308984&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>

## 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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