

# 13-Chloropentadecanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C16H31ClO2/c1-3-15(17)13-11-9-7-5-4-6-8-10-12-14-16(18)19-2/h15H,3-14H2
<b>InchiKey:</b>	LRNFIVRAPNCJHV-UHFFFAOYSA-N
<b>Formula:</b>	C16H31ClO2
<b>SMILES:</b>	CCC(Cl)CCCCCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	290.87

## Physical Properties

Property code	Value	Unit	Source
gf	-164.45	kJ/mol	Joback Method
hf	-639.39	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.468		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2506.00		NIST Webbook
tb	678.76	K	Joback Method
tc	853.20	K	Joback Method
tf	357.16	K	Joback Method
vc	0.999	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.02	J/molxK	678.76	Joback Method
cpg	789.95	J/molxK	824.12	Joback Method
cpg	775.70	J/molxK	795.05	Joback Method
cpg	760.71	J/molxK	765.98	Joback Method
cpg	744.94	J/molxK	736.91	Joback Method
cpg	728.39	J/molxK	707.83	Joback Method

cpg	803.46	J/mol×K	853.20	Joback Method
dvisc	0.0001020	Paxs	678.76	Joback Method
dvisc	0.0001380	Paxs	625.16	Joback Method
dvisc	0.0001977	Paxs	571.56	Joback Method
dvisc	0.0003050	Paxs	517.96	Joback Method
dvisc	0.0005200	Paxs	464.36	Joback Method
dvisc	0.0010191	Paxs	410.76	Joback Method
dvisc	0.0024442	Paxs	357.16	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=R308964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308964&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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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