

# 3-Chlorohexadecanoic acid, methyl ester

**Inchi:** InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-16(18)15-17(19)20-2/h16H,3-15H  
**InchiKey:** ZWSOWVGTXJXORW-UHFFFAOYSA-N  
**Formula:** C17H33ClO2  
**SMILES:** CCCCCCCCCCCCCC(Cl)CC(=O)OC  
**Mol. weight [g/mol]:** 304.90

## Physical Properties

Property code	Value	Unit	Source
gf	-156.03	kJ/mol	Joback Method
hf	-660.03	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.858		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2062.00		NIST Webbook
ripol	2485.00		NIST Webbook
ripol	2490.00		NIST Webbook
tb	701.64	K	Joback Method
tc	876.28	K	Joback Method
tf	368.43	K	Joback Method
vc	1.054	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.83	J/molxK	701.64	Joback Method
cpg	848.48	J/molxK	847.17	Joback Method
cpg	833.96	J/molxK	818.07	Joback Method
cpg	818.65	J/molxK	788.96	Joback Method
cpg	802.54	J/molxK	759.85	Joback Method
cpg	785.61	J/molxK	730.75	Joback Method

cpg	862.24	J/mol×K	876.28	Joback Method
dvisc	0.0000893	Paxs	701.64	Joback Method
dvisc	0.0001212	Paxs	646.11	Joback Method
dvisc	0.0001741	Paxs	590.57	Joback Method
dvisc	0.0002695	Paxs	535.03	Joback Method
dvisc	0.0004619	Paxs	479.50	Joback Method
dvisc	0.0009117	Paxs	423.97	Joback Method
dvisc	0.0022085	Paxs	368.43	Joback Method

## Sources

<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>
<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=R309249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R309249&amp;Units=SI</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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