

# 3-Chloroheptadecanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C18H35ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-17(19)16-18(20)21-2/h17H,1-16H,2H
<b>InchiKey:</b>	XUDZISROSCNUMV-UHFFFAOYSA-N
<b>Formula:</b>	C18H35ClO2
<b>SMILES:</b>	CCCCCCCCCCCC(CI)CC(=O)OC
<b>Mol. weight [g/mol]:</b>	318.92

## Physical Properties

Property code	Value	Unit	Source
gf	-147.61	kJ/mol	Joback Method
hf	-680.67	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	6.248		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpola	2169.00		NIST Webbook
ripola	2592.00		NIST Webbook
tb	724.52	K	Joback Method
tc	899.87	K	Joback Method
tf	379.70	K	Joback Method
vc	1.111	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.77	J/molxK	724.52	Joback Method
cpg	908.06	J/molxK	870.64	Joback Method
cpg	893.27	J/molxK	841.42	Joback Method
cpg	877.67	J/molxK	812.19	Joback Method
cpg	861.23	J/molxK	782.97	Joback Method
cpg	843.94	J/molxK	753.74	Joback Method
cpg	922.05	J/molxK	899.87	Joback Method
dvisc	0.0000780	Paxs	724.52	Joback Method

dvisc	0.0001060	Paxs	667.05	Joback Method
dvisc	0.0001527	Paxs	609.58	Joback Method
dvisc	0.0002373	Paxs	552.11	Joback Method
dvisc	0.0004087	Paxs	494.64	Joback Method
dvisc	0.0008119	Paxs	437.17	Joback Method
dvisc	0.0019853	Paxs	379.70	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R309229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R309229&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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