

# 12-Chlorooctadecanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C19H37ClO2/c1-3-4-5-12-15-18(20)16-13-10-8-6-7-9-11-14-17-19(21)22-2/h18
<b>InchiKey:</b>	FPYBFYPWERLQGZ-UHFFFAOYSA-N
<b>Formula:</b>	C19H37ClO2
<b>SMILES:</b>	CCCCCCC(Cl)CCCCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	332.95

## Physical Properties

Property code	Value	Unit	Source
gf	-139.19	kJ/mol	Joback Method
hf	-701.31	kJ/mol	Joback Method
hfus	48.43	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.638		Crippen Method
mvol	298.250	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
tb	747.40	K	Joback Method
tc	924.01	K	Joback Method
tf	390.97	K	Joback Method
vc	1.167	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.74	J/molxK	747.40	Joback Method
cpg	903.32	J/molxK	776.83	Joback Method
cpg	920.97	J/molxK	806.27	Joback Method
cpg	937.72	J/molxK	835.70	Joback Method
cpg	953.60	J/molxK	865.14	Joback Method
cpg	968.63	J/molxK	894.57	Joback Method
cpg	982.84	J/molxK	924.01	Joback Method
dvisc	0.0017764	Paxs	390.97	Joback Method
dvisc	0.0007200	Paxs	450.38	Joback Method
dvisc	0.0003602	Paxs	509.78	Joback Method

dvisc	0.0002082	Paxs	569.18	Joback Method
dvisc	0.0001335	Paxs	628.59	Joback Method
dvisc	0.0000924	Paxs	687.99	Joback Method
dvisc	0.0000678	Paxs	747.40	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=R308895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308895&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>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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