

# 6,9,12-Octadecatrienoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C19H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-
<b>InchiKey:</b>	JFRWATCOFCPIBM-SPOHZTNBSA-N
<b>Formula:</b>	C19H32O2
<b>SMILES:</b>	CCCCC=CCC=CC=CCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	292.46
<b>CAS:</b>	2676-41-7

## Physical Properties

Property code	Value	Unit	Source
gf	115.84	kJ/mol	Joback Method
hf	-328.63	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.749		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
tb	722.89	K	Joback Method
tc	904.64	K	Joback Method
tf	360.81	K	Joback Method
vc	1.063	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.46	J/molxK	722.89	Joback Method
cpg	798.24	J/molxK	753.18	Joback Method
cpg	815.15	J/molxK	783.47	Joback Method
cpg	831.25	J/molxK	813.77	Joback Method
cpg	846.59	J/molxK	844.06	Joback Method
cpg	861.21	J/molxK	874.35	Joback Method
cpg	875.18	J/molxK	904.64	Joback Method
dvisc	0.0015069	Paxs	360.81	Joback Method
dvisc	0.0005818	Paxs	421.16	Joback Method

dvisc	0.0002851	Paxs	481.50	Joback Method
dvisc	0.0001638	Paxs	541.85	Joback Method
dvisc	0.0001052	Paxs	602.20	Joback Method
dvisc	0.0000732	Paxs	662.54	Joback Method
dvisc	0.0000541	Paxs	722.89	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2676417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2676417&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>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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