

# 9,12-Octadecadiynoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C19H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h3-6,9,11-14,17-18,20,21
<b>InchiKey:</b>	VATNVLNGBAFLPT-UHFFFAOYSA-N
<b>Formula:</b>	C19H30O2
<b>SMILES:</b>	CCCCC#CCC#CCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	290.44

## Physical Properties

Property code	Value	Unit	Source
gf	280.78	kJ/mol	Joback Method
hf	-135.69	kJ/mol	Joback Method
hfus	54.00	kJ/mol	Joback Method
hvap	71.35	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.867		Crippen Method
mvol	268.810	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2208.80		NIST Webbook
tb	728.41	K	Joback Method
tc	922.41	K	Joback Method
tf	588.25	K	Joback Method
vc	1.048	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.45	J/mol×K	728.41	Joback Method
cpg	777.66	J/mol×K	760.74	Joback Method
cpg	794.94	J/mol×K	793.08	Joback Method
cpg	811.30	J/mol×K	825.41	Joback Method
cpg	826.77	J/mol×K	857.74	Joback Method
cpg	841.38	J/mol×K	890.08	Joback Method
cpg	855.14	J/mol×K	922.41	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=U333564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333564&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-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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