

# 6-Octadecenoic acid, methyl ester, (Z)-

<b>Other names:</b>	Methyl cis-6-octadecenoate Methyl petroselinate cis-6-Octadecenoic acid, methyl ester methyl (Z)-octadec-6-enoate
<b>Inchi:</b>	InChI=1S/C19H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h13-14H
<b>InchiKey:</b>	QRTVDKVXAFJVRU-YPKPFQOOSA-N
<b>Formula:</b>	C19H36O2
<b>SMILES:</b>	CCCCCCCCCCC=CCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	296.49
<b>CAS:</b>	2777-58-4

## Physical Properties

Property code	Value	Unit	Source
gf	-44.60	kJ/mol	Joback Method
hf	-563.07	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.197		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2104.50		NIST Webbook
tb	714.57	K	Joback Method
tc	887.77	K	Joback Method
tf	370.97	K	Joback Method
vc	1.103	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.19	J/molxK	714.57	Joback Method
cpg	844.92	J/molxK	743.44	Joback Method
cpg	862.78	J/molxK	772.30	Joback Method
cpg	879.80	J/molxK	801.17	Joback Method

cpg	896.00	J/molxK	830.04	Joback Method
cpg	911.43	J/molxK	858.90	Joback Method
cpg	926.09	J/molxK	887.77	Joback Method
dvisc	0.0017193	Paxs	370.97	Joback Method
dvisc	0.0007124	Paxs	428.24	Joback Method
dvisc	0.0003634	Paxs	485.50	Joback Method
dvisc	0.0002137	Paxs	542.77	Joback Method
dvisc	0.0001390	Paxs	600.04	Joback Method
dvisc	0.0000975	Paxs	657.30	Joback Method
dvisc	0.0000724	Paxs	714.57	Joback Method

## Sources

<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=C2777584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2777584&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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