

# Octadecanoic acid, 12-oxo-, methyl ester

<b>Other names:</b>	Methyl 12-ketostearate Methyl 12-oxostearate 12-Oxostearic acid, methyl ester
<b>Inchi:</b>	InChI=1S/C19H36O3/c1-3-4-5-12-15-18(20)16-13-10-8-6-7-9-11-14-17-19(21)22-2/h3-17
<b>InchiKey:</b>	XVSPEBNRFAFNAV-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O3
<b>SMILES:</b>	CCCCCCC(=O)CCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	312.49
<b>CAS:</b>	2380-27-0

## Physical Properties

Property code	Value	Unit	Source
gf	-253.74	kJ/mol	Joback Method
hf	-792.87	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.600		Crippen Method
mcvol	287.580	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
tb	764.28	K	Joback Method
tc	942.71	K	Joback Method
tf	425.98	K	Joback Method
vc	1.129	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.43	J/molxK	764.28	Joback Method
cpg	895.45	J/molxK	794.02	Joback Method
cpg	912.55	J/molxK	823.76	Joback Method
cpg	928.74	J/molxK	853.50	Joback Method
cpg	944.06	J/molxK	883.24	Joback Method
cpg	958.51	J/molxK	912.98	Joback Method

cpg	972.13	J/molxK	942.71	Joback Method
dvisc	0.0013667	Paxs	425.98	Joback Method
dvisc	0.0006490	Paxs	482.36	Joback Method
dvisc	0.0003602	Paxs	538.75	Joback Method
dvisc	0.0002235	Paxs	595.13	Joback Method
dvisc	0.0001506	Paxs	651.51	Joback Method
dvisc	0.0001081	Paxs	707.90	Joback Method
dvisc	0.0000815	Paxs	764.28	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.20	K	0.10	NIST Webbook

## 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=C2380270&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2380270&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>
<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

**tbrp:** Boiling point at reduced pressure  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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