9-Octadecenoic acid, methyl ester

Other names:	Methyl 9-octadecenoate
	18:1n-9 methyl ester
	Methyl octadec-9-enoate
Inchi:	InChI=1S/C19H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h10-11H
InchiKey:	QYDYPVFESGNLHU-ZHACJKMWSA-N
Formula:	C19H36O2
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	296.49
CAS:	2462-84-2

Physical Properties

Property code	Value	Unit	Source
chl	-11852.00	kJ/mol	NIST Webbook
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	2107.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2101.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2466.00		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/mol×K	714.57	Joback Method
cpg	844.92	J/mol×K	743.44	Joback Method
cpg	862.78	J/mol×K	772.30	Joback Method
cpg	879.80	J/mol×K	801.17	Joback Method
cpg	896.00	J/mol×K	830.04	Joback Method
cpg	911.43	J/mol×K	858.90	Joback Method
cpg	926.09	J/mol×K	887.77	Joback Method
dvisc	0.0017193	Pa×s	370.97	Joback Method
dvisc	0.0007124	Pa×s	428.24	Joback Method
dvisc	0.0003634	Pa×s	485.50	Joback Method
dvisc	0.0002137	Pa×s	542.77	Joback Method
dvisc	0.0001390	Pa×s	600.04	Joback Method
dvisc	0.0000975	Pa×s	657.30	Joback Method
dvisc	0.0000724	Pa×s	714.57	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2462842&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume