11-Octadecenoic acid, methyl ester

Other names:	Methyl 11-octadecenoate
	Octadec-11-enoic acid, methyl ester
	trans-Vaccenic acid, methyl ester
	16:1n-7 methyl ester
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/h8-9H,3-
InchiKey:	PVVODBCDJBGMJL-CMDGGOBGSA-N
Formula:	C19H36O2
SMILES:	CCCCCCC=CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	296.49
CAS:	52380-33-3

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	2089.00		NIST Webbook
rinpol	2115.20		NIST Webbook
rinpol	2089.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52380333&Units=SI
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

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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