Methyl hexadec-9-enoate

Other names:	Methyl palmitelaidate
	(E)-9-hexadecenoic acid methyl ester
	9-Hexadecenoic acid, (E), methyl ester
	Methyl trans-9-hexadecenoate
Inchi:	InChI=1S/C17H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h8-9H,3-7,10-1
InchiKey:	IZFGRAGOVZCUFB-CMDGGOBGSA-N
Formula:	C17H32O2
SMILES:	CCCCCCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	268.43
CAS:	10030-74-7

Physical Properties

Property code	Value	Unit	Source
gf	-61.44	kJ/mol	Joback Method
hf	-521.79	kJ/mol	Joback Method
hfl	-665.38	kJ/mol	NIST Webbook
hfus	42.77	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1907.00		NIST Webbook
rinpol	317.66		NIST Webbook
rinpol	1916.70		NIST Webbook
rinpol	317.66		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1916.70		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1895.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2237.00		NIST Webbook
tb	668.81	K	Joback Method
tc	841.03	K	Joback Method
tf	348.43	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/mol×K	668.81	Joback Method
cpg	792.67	J/mol×K	812.33	Joback Method
cpg	777.84	J/mol×K	783.62	Joback Method
cpg	762.28	J/mol×K	754.92	Joback Method
cpg	745.96	J/mol×K	726.22	Joback Method
cpg	728.86	J/mol×K	697.51	Joback Method
cpg	806.79	J/mol×K	841.03	Joback Method
dvisc	0.0000930	Pa×s	668.81	Joback Method
dvisc	0.0001246	Pa×s	615.41	Joback Method
dvisc	0.0001766	Pa×s	562.02	Joback Method
dvisc	0.0002691	Pa×s	508.62	Joback Method
dvisc	0.0004527	Pa×s	455.22	Joback Method
dvisc	0.0008745	Pa×s	401.83	Joback Method
dvisc	0.0020673	Pa×s	348.43	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=C10030747&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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