9,12-Octadecadienoic acid, methyl ester

Other names:	9,12-Octadecenoic acid, methyl ester
	Methyl octadeca-9,12-dienoate
	Methyl 9,12-octadecadienoate
	9,12-Octadecadienoic acid
	octadeca-9,12-dienoic acid
Inchi:	InChI=1S/C19H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-
InchiKey:	WTTJVINHCBCLGX-UHFFFAOYSA-N
Formula:	C19H34O2
SMILES:	CCCCCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	294.47
CAS:	2462-85-3

Physical Properties

Property code	Value	Unit	Source
gf	35.62	kJ/mol	Joback Method
hf	-445.85	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	66.96	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.973		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2092.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	356.30		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2092.00		NIST Webbook
rinpol	2069.00		NIST Webbook

rinpol	356.30		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2101.00		NIST Webbook
ripol	2472.00		NIST Webbook
ripol	2478.00		NIST Webbook
tb	718.73	K	Joback Method
tc	896.01	K	Joback Method
tf	365.89	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.45	J/mol×K	718.73	Joback Method
cpg	821.70	J/mol×K	748.28	Joback Method
cpg	839.08	J/mol×K	777.82	Joback Method
cpg	855.63	J/mol×K	807.37	Joback Method
cpg	871.40	J/mol×K	836.92	Joback Method
cpg	886.41	J/mol×K	866.47	Joback Method
cpg	900.71	J/mol×K	896.01	Joback Method
dvisc	0.0016090	Pa×s	365.89	Joback Method
dvisc	0.0006439	Pa×s	424.70	Joback Method
dvisc	0.0003219	Pa×s	483.50	Joback Method
dvisc	0.0001871	Pa×s	542.31	Joback Method
dvisc	0.0001209	Pa×s	601.12	Joback Method
dvisc	0.0000845	Pa×s	659.92	Joback Method
dvisc	0.0000626	Pa×s	718.73	Joback Method

Sources

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=C2462853&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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