

9,12-Octadecadienoic acid, methyl ester, (E,E)-

Other names:

Linolelaidic acid, methyl ester
Methyl linolelaidate
Methyl trans,trans-9,12-octadecadienoate
Methyl 9-trans-12-trans-octadecadienoate
Methyl (E, E)-9,12-octadecadienoate
trans-9,12-Octadecadienoic acid, methyl ester
methyl (9E,12E)-octadeca-9,12-dienoate

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-ZDVGBALWSA-N**Formula:** C19H34O2**SMILES:** CCCCCC=CCC=CCCCCCCCC(=O)OC**Mol. weight [g/mol]:** 294.47**CAS:** 2566-97-4

Physical Properties

Property code	Value	Unit	Source
gf	35.62	kJ/mol	Joback Method
hf	-445.85	kJ/mol	Joback Method
hfl	-617.01	kJ/mol	NIST Webbook
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	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
ripol	2405.00		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/molxK	718.73	Joback Method
cpg	886.41	J/molxK	866.47	Joback Method
cpg	871.40	J/molxK	836.92	Joback Method
cpg	855.63	J/molxK	807.37	Joback Method
cpg	839.08	J/molxK	777.82	Joback Method
cpg	821.70	J/molxK	748.28	Joback Method
cpg	900.71	J/molxK	896.01	Joback Method
dvisc	0.0000626	Paxs	718.73	Joback Method
dvisc	0.0000845	Paxs	659.92	Joback Method
dvisc	0.0001209	Paxs	601.12	Joback Method
dvisc	0.0001871	Paxs	542.31	Joback Method
dvisc	0.0003219	Paxs	483.50	Joback Method
dvisc	0.0006439	Paxs	424.70	Joback Method
dvisc	0.0016090	Paxs	365.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2566974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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