

2,6-Nonadienoic acid, 9-(3,3-dimethyloxiranyl)-3,7-dimethyl-, methyl ester, (E,E)-

Other names: 2,6-Dodecadienoic acid, 10,11-epoxy-3,7,11-trimethyl-, methyl ester, (E,E)-trans-trans-10,11-Epoxyfarnesenic acid methyl ester

Juvenate

Juvenile hormone C16

Methyl trans,trans-10,11-epoxyfarnesoate

SJH I

(E,E)-Methyl-10,11-epoxyfarnesoate

Inchi: InChI=1S/C16H26O3/c1-12(9-10-14-16(3,4)19-14)7-6-8-13(2)11-15(17)18-5/h7,11,14H,6

InchiKey: QVJMXSGZTCGLHZ-ZPLWXOMKSA-N

Formula: C16H26O3

SMILES: COC(=O)C=C(C)CCC=C(C)CCC1OC1(C)C

Mol. weight [g/mol]: 266.38

CAS: 5299-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-45.31	kJ/mol	Joback Method
hf	-467.81	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	63.41	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.790		Crippen Method
mcvol	230.150	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
tb	679.11	K	Joback Method
tc	877.08	K	Joback Method
tf	368.33	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	651.71	J/mol×K	679.11	Joback Method
cpg	669.25	J/mol×K	712.10	Joback Method
cpg	686.03	J/mol×K	745.10	Joback Method
cpg	702.19	J/mol×K	778.09	Joback Method
cpg	717.84	J/mol×K	811.09	Joback Method
cpg	733.11	J/mol×K	844.08	Joback Method
cpg	748.12	J/mol×K	877.08	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=C5299116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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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