2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester

Other names: Methyl geranate
Methyl geraniate
Methyl 3,7-dimethyl-2,6-octadienoate

Inchi: InChI=1S/C11H18O2/c1-9(2)6-5-7-10(3)8-11(12)13-4/h6,8H,5,7H2,1-4H3/b10-8+

InchiKey: ACOBBFVLNKYODD-CSKARUKUSA-N

Formula: C11H18O2

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

Mol. weight [g/mol]: 182.26

CAS: 2349-14-6

Physical Properties

Property code	Value	Unit	Source
gf	-48.84	kJ/mol	Joback Method
hf	-300.31	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1305.00		NIST Webbook

rinpol	1323.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1302.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1701.00		NIST Webbook
tb	535.45	K	Joback Method
tc	727.53	K	Joback Method
tf	247.81	K	Joback Method

vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.86	J/mol×K	535.45	Joback Method
cpg	393.51	J/mol×K	567.46	Joback Method
cpg	407.43	J/mol×K	599.48	Joback Method
cpg	420.66	J/mol×K	631.49	Joback Method
cpg	433.22	J/mol×K	663.51	Joback Method
cpg	445.15	J/mol×K	695.52	Joback Method
cpg	456.47	J/mol×K	727.53	Joback Method

Sources

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=C2349146&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

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