trans-Geranic acid methyl ester

Other names:	2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester, (E)-
	E-Methylgeranate
	Geranic acid methyl ester
	Methyl geranoate
	Methyl trans-geranate
	Methyl geranate
	Methyl (2E)-3,7-dimethyl-2,6-octadienoate
	(E)-Geranic acid methyl ester
	Methyl 2,6-octadienoate, 3,7-dimethyl, (E)-
	Methyl (E)-2,6-octadienoate, 3,7-dimethyl
	Methyl E-geranate
	Methyl (E)-geraniate
	2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester, (2E)-
	methyl (E)-3,7-dimethylocta-2,6-dienoate
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:	1189-09-9

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	1321.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1302.00		NIST Webbook

rinpol	1321.70		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1321.70		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1679.00		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

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=C1189099&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
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