Geranyl tiglate

Other names: 2-Butenoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E,E)-
2,6-Octadien-1-ol, 3,7-dimethyl-, 2-methyl-2-butenoate, (E,E)--
cis-«alpha»,«beta»-Dimethyl acrylic acid, geraniol ester
trans-3,7-Dimethyl-2,6-octadien-1-yl cis-«alpha»,«beta»-dimethyl acrylate
Tiglic acid, geraniol ester
(2E)-3,7-Dimethyl-2,6-octadienyl (2E)-2-methyl-2-butenoate
(E)-(E)-3,7-Dimethylocta-2,6-dien-1-yl 2-methylbut-2-enoate
(E)-3,7-Dimethylocta-2,6-dienyl (E)-2-methylbut-2-enoate
Gernyl tiglate
Geranyl (E)-2-methyl-2-butenoate
(E)-3,7-dimethyl-2,6-octadienyl 2-methylcrotonate

Inchi: InChI=1S/C15H24O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h6,8,10H,7,9,11H2,1-

InchiKey: OGHBUHJLMHQMHS-KRDNBFTESA-N

Formula: C15H24O2

SMILES: CC=C(C)C(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 236.35

CAS: 7785-33-3

Physical Properties

Property code	Value	Unit	Source
gf	56.51	kJ/mol	Joback Method
hf	-275.44	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.189		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1704.00		NIST Webbook

rinpol	1705.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1675.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2109.00		NIST Webbook
tb	631.01	K	Joback Method
tc	824.40	K	Joback Method
tf	273.85	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.71	J/mol×K	631.01	Joback Method
cpg	575.50	J/mol×K	663.24	Joback Method
cpg	591.43	J/mol×K	695.47	Joback Method
cpg	606.52	J/mol×K	727.71	Joback Method
cpg	620.85	J/mol×K	759.94	Joback Method
cpg	634.44	J/mol×K	792.17	Joback Method
cpg	647.37	J/mol×K	824.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7785333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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