Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-

Other names:	Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
	Geranyl isobutyrate
	Isobutyric acid, (E)-3,7-dimethyl-2,6-octadienyl ester
	3,7-Dimethyl-2,6-octadienyl isobutyrate
	Propionic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester,
	trans-3-7-Dimethyl-2,6-octadienyl isobutyrate
	Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, trans-
	2,6-Octadien-1-ol, 3,7-dimethyl-, isobutyrate, trans-
	Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester,
	3,7-Dimethyl-2,6-octadienyl isobutyrate, (E)-
	Propionic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, trans-
	Propanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, trans-
	Geranyl 2-methylpropanoate
	Geranyl isobutanoate
	Geraniol isobutyrate
	Propanoic acid, 2-methyl-, (2E)-3,7-dimethyl-2,6-octadien-1-yl ester
	Propanoic acid, 2-methyl-, (2E)-3,7-dimethyl-2,6-octadienyl ester
Inchi:	InChI=1S/C14H24O2/c1-11(2)7-6-8-13(5)9-10-16-14(15)12(3)4/h7,9,12H,6,8,10H2,1-5H3
InchiKey:	OGJYXQFXLSCKTP-LCYFTJDESA-N
Formula:	C14H24O
SMILES:	CC(C)=CCCC(C)=CCOC(=O)C(C)C
Mol. weight [g/mol]:	208.34
CAS:	2345-26-8

Physical Properties

Property code	Value	Unit	Source
gf	-26.02	kJ/mol	Joback Method
hf	-367.51	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1491.00		NIST Webbook

rinpol	1493.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1515.60		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1514.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1821.00		NIST Webbook
tb	603.65	K	Joback Method
tc	792.58	K	Joback Method
tf	266.62	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.86	J/mol×K	761.09	Joback Method
cpg	527.51	J/mol×K	603.65	Joback Method
cpg	544.38	J/mol×K	635.14	Joback Method
cpg	560.42	J/mol×K	666.63	Joback Method

cpg	575.66	J/mol×K	698.11	Joback Method
cpg	590.12	J/mol×K	729.60	Joback Method
cpg	616.90	J/mol×K	792.58	Joback Method
hvapt	67.80	kJ/mol	443.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2345268&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
hvapt:	Enthalpy of vaporization at a given temperature
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