Geranyl propionate

Other names:	2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (E)-
	2,6-Octadien-1-ol, 3,7-dimethyl-, propionate, (E)-
	trans-3,7-Dimethyl-2,6-octadienyl propionate
	Geranyl n-propionate
	Geranyl n-propanoate
	Geranyl propanoate
	(2E)-3,7-Dimethyl-2,6-octadienyl propionate
	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-propanoate, (2E)-
	Propionic acid, geranyl ester
	(E)-3,7-Dimethyl-2,6-octadien-1-ol propanoate
	2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (2E)-
Inchi:	InChI=1S/C13H22O2/c1-5-13(14)15-10-9-12(4)8-6-7-11(2)3/h7,9H,5-6,8,10H2,1-4H3/b12
InchiKey:	BYCHQEILESTMQU-FMIVXFBMSA-N
Formula:	C13H22O2
SMILES:	CCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	210.31
CAS:	105-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-32.00	kJ/mol	Joback Method
hf	-341.59	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1475.00		NIST Webbook

rinpol	1452.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1485.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1450.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1487.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1449.80	NIST Webbook
rinpol	1449.00	NIST Webbook
rinpol	1453.00	NIST Webbook
rinpol	1448.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1449.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1448.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1476.00	NIST Webbook
rinpol	1451.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1473.00	NIST Webbook
ripol	1799.00	NIST Webbook
ripol	1819.00	NIST Webbook
ripol	1812.00	NIST Webbook
ripol	1817.00	NIST Webbook
ripol	1819.00	NIST Webbook
ripol	1800.00	NIST Webbook
ripol	1834.00	NIST Webbook
ripol	1817.00	NIST Webbook
ripol	1812.00	NIST Webbook
ripol	1827.00	NIST Webbook
ripol	1827.00	NIST Webbook
ripol	1830.00	NIST Webbook

ripol	1828.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1823.00		NIST Webbook
tb	581.21	K	Joback Method
tc	768.75	K	Joback Method
tf	270.35	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.11	J/mol×K	581.21	Joback Method
cpg	492.09	J/mol×K	612.47	Joback Method
cpg	507.29	J/mol×K	643.72	Joback Method
cpg	521.75	J/mol×K	674.98	Joback Method
cpg	535.49	J/mol×K	706.24	Joback Method
cpg	548.55	J/mol×K	737.49	Joback Method
cpg	560.96	J/mol×K	768.75	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105908&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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