Geranyl isovalerate

Other names: Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-
2,6-Octadien-1-ol, 3,7-dimethyl-, isovalerate, (E)-
Butyric acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-
trans-3,7-Dimethyl-2,6-octadienyl isopentanoate
Isovaleric acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
Geranyl 3-methylbutanoate
Geranyl isopentanoate

Inchi: InChI=1S/C15H26O2/c1-12(2)7-6-8-14(5)9-10-17-15(16)11-13(3)4/h7,9,13H,6,8,10-11H2

InchiKey: SOUKTGNMIRUIQN-NTEUORMPSA-N

Formula: C15H26O2

SMILES: CC(C)=CCCC(C)=CCOC(=O)CC(C)C

Mol. weight [g/mol]: 238.37

CAS: 109-20-6

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1605.00		NIST Webbook

rinpol	1582.00		NIST Webbook
rinpol	1610.70		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1593.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1919.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1925.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1913.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method

cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109206&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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