

Geranyl acetate

Other names:	(2E)-3,7-Dimethyl-2,6-octadienyl acetate (E)-3,7-Dimethyl-2,6-octadien-1-ol acetate (E)-3,7-Dimethyl-2,6-octadien-1-yl acetate 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (2E)- 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)- 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, trans- 3,7-Dimethyl-2-trans, 6-octadienyl acetate Acetic acid, geraniol ester Bay pine (oyster) oil Geraniol acetate Geranyl ethanoate Meraneine NCI-C54728 NSC 2584 trans-2,6-Dimethyl-2,6-octadien-8-yl ethanoate trans-3,7-Dimethyl-2,6-octadien-1-ol, acetate trans-3,7-Dimethyl-2,6-octadien-1-yl acetate trans-Geranyl acetate
Inchi:	InChI=1S/C12H20O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6,8H,5,7,9H2,1-4H3/b11-8+
InchiKey:	HIGQPQRQIQDZMP-DHZHZOJOSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	196.29
CAS:	105-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-40.42	kJ/mol	Joback Method
hf	-320.95	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	51.54	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
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ripol	1765.00	NIST Webbook

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tb	558.33	K	Joback Method
tc	748.06	K	Joback Method
tf	259.08	K	Joback Method
vc	0.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.22	J/mol×K	716.44	Joback Method
cpg	426.65	J/mol×K	558.33	Joback Method
cpg	442.01	J/mol×K	589.95	Joback Method
cpg	456.62	J/mol×K	621.57	Joback Method
cpg	470.50	J/mol×K	653.20	Joback Method
cpg	483.69	J/mol×K	684.82	Joback Method
cpg	508.12	J/mol×K	748.06	Joback Method
hvapt	58.10	kJ/mol	431.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.73185e+01
Coeff. B	-6.41278e+03
Coeff. C	-1.16860e+01
Temperature range (K), min.	388.22
Temperature range (K), max.	545.77

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105873&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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