

# Geranyl isoctanoate

<b>Inchi:</b>	InChI=1S/C18H32O2/c1-15(2)9-6-7-12-18(19)20-14-13-17(5)11-8-10-16(3)4/h10,13,15H
<b>InchiKey:</b>	JSKBFQNICWTSJO-LGMDPLHJSA-N
<b>Formula:</b>	C18H32O2
<b>SMILES:</b>	CC(C)=CCCC(C)=CCOC(=O)CCCCC(C)C
<b>Mol. weight [g/mol]:</b>	280.45

## Physical Properties

Property code	Value	Unit	Source
gf	7.66	kJ/mol	Joback Method
hf	-450.07	kJ/mol	Joback Method
hfus	39.42	kJ/mol	Joback Method
hvap	64.51	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.439		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
tb	695.17	K	Joback Method
tc	878.37	K	Joback Method
tf	311.70	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.63	J/mol×K	695.17	Joback Method
cpg	764.10	J/mol×K	725.70	Joback Method
cpg	781.67	J/mol×K	756.24	Joback Method
cpg	798.37	J/mol×K	786.77	Joback Method
cpg	814.25	J/mol×K	817.30	Joback Method
cpg	829.35	J/mol×K	847.84	Joback Method
cpg	843.70	J/mol×K	878.37	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R200687&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R200687&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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