

# Farnesyl octanoate, (E,E)-

<b>Inchi:</b>	InChI=1S/C23H40O2/c1-6-7-8-9-10-17-23(24)25-19-18-22(5)16-12-15-21(4)14-11-13-20
<b>InchiKey:</b>	HHSVAJNBWYMLPB-QMEDZHDISA-N
<b>Formula:</b>	C23H40O2
<b>SMILES:</b>	CCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	348.56

## Physical Properties

Property code	Value	Unit	Source
gf	123.87	kJ/mol	Joback Method
hf	-440.56	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	76.06	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.309		Crippen Method
mcvol	329.470	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
ripol	2373.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2669.00		NIST Webbook
ripol	2669.00		NIST Webbook
tb	814.05	K	Joback Method
tc	1003.63	K	Joback Method
tf	364.01	K	Joback Method
vc	1.290	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.65	J/molxK	814.05	Joback Method
cpg	1037.32	J/molxK	845.65	Joback Method
cpg	1056.02	J/molxK	877.24	Joback Method
cpg	1073.84	J/molxK	908.84	Joback Method
cpg	1090.84	J/molxK	940.44	Joback Method

cpg	1107.08	J/mol×K	972.03	Joback Method
cpg	1122.63	J/mol×K	1003.63	Joback Method

## Sources

<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=R66401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R66401&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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>hvap:</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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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