

# dehydrovomifoliol

<b>Inchi:</b>	InChI=1S/C13H18O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h7,10,14,16H,8H2,1-4H
<b>InchiKey:</b>	GGJZTVFPVNUUIZ-GWCFXTLKSA-N
<b>Formula:</b>	C13H18O3
<b>SMILES:</b>	CC1=CC(=O)CC(C)(C)C1(O)C#CC(C)O
<b>Mol. weight [g/mol]:</b>	222.28

## Physical Properties

Property code	Value	Unit	Source
gf	-111.20	kJ/mol	Joback Method
hf	-376.02	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.047		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1765.00		NIST Webbook
ripol	3067.00		NIST Webbook
ripol	3067.00		NIST Webbook
ripol	3065.00		NIST Webbook
tb	777.08	K	Joback Method
tc	994.49	K	Joback Method
tf	581.45	K	Joback Method
vc	0.678	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	543.31	J/mol×K	777.08	Joback Method
cpg	558.06	J/mol×K	813.31	Joback Method
cpg	572.82	J/mol×K	849.55	Joback Method
cpg	587.77	J/mol×K	885.78	Joback Method
cpg	603.06	J/mol×K	922.02	Joback Method
cpg	618.88	J/mol×K	958.25	Joback Method
cpg	635.37	J/mol×K	994.49	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R223259&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R223259&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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