

# neo-isopulegol acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3/t9
<b>InchiKey:</b>	HLHIVJRLSDSUCI-USWWRNFRSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	C=C(C)C1CCC(C)CC1OC(C)=O
<b>Mol. weight [g/mol]:</b>	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-95.44	kJ/mol	Joback Method
hf	-406.53	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1298.00		NIST Webbook
tb	557.02	K	Joback Method
tc	763.76	K	Joback Method
tf	280.34	K	Joback Method
vc	0.644	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.53	J/molxK	557.02	Joback Method
cpg	455.28	J/molxK	591.48	Joback Method
cpg	474.03	J/molxK	625.93	Joback Method
cpg	491.78	J/molxK	660.39	Joback Method
cpg	508.54	J/molxK	694.85	Joback Method

cpg	524.33	J/mol×K	729.31	Joback Method
cpg	539.15	J/mol×K	763.76	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=R235975&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235975&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.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>rinpolar:</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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