

# neo-Isopulegyl acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,12H,5-7H2,1-4H3
<b>InchiKey:</b>	ZAPTZQHAWAYFSW-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	CC(=O)OC1CC(C)CCC1=C(C)C
<b>Mol. weight [g/mol]:</b>	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-130.11	kJ/mol	Joback Method
hf	-435.59	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinsol	1263.00		NIST Webbook
tb	571.65	K	Joback Method
tc	780.75	K	Joback Method
tf	296.70	K	Joback Method
vc	0.647	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.34	J/mol×K	571.65	Joback Method
cpg	455.18	J/mol×K	606.50	Joback Method
cpg	473.04	J/mol×K	641.35	Joback Method
cpg	489.95	J/mol×K	676.20	Joback Method
cpg	505.91	J/mol×K	711.05	Joback Method
cpg	520.93	J/mol×K	745.90	Joback Method
cpg	535.03	J/mol×K	780.75	Joback Method

# Sources

<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=R410785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R410785&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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