

# isopimarinol

**Inchi:** InChI=1S/C20H32O/c1-5-18(2)12-9-16-15(13-18)7-8-17-19(3,14-21)10-6-11-20(16,17)4/  
**InchiKey:** DUEINKIQNGZKPL-WAPOTWQKSA-N  
**Formula:** C20H32O  
**SMILES:** C=CC1(C)CCC2C(=CCC3C(C)(CO)CCCC23C)C1  
**Mol. weight [g/mol]:** 288.47

## Physical Properties

Property code	Value	Unit	Source
gf	178.73	kJ/mol	Joback Method
hf	-243.98	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.114		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	782.95	K	Joback Method
tc	1004.60	K	Joback Method
tf	486.94	K	Joback Method
vc	0.965	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.59	J/mol×K	782.95	Joback Method
cpg	865.45	J/mol×K	819.89	Joback Method
cpg	889.43	J/mol×K	856.83	Joback Method
cpg	913.91	J/mol×K	893.78	Joback Method
cpg	939.25	J/mol×K	930.72	Joback Method
cpg	965.82	J/mol×K	967.66	Joback Method
cpg	993.99	J/mol×K	1004.60	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=R167203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R167203&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>h vap:</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>r in pol:</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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