

# epi-Cubebol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-9(2)11-6-5-10(3)15-8-7-14(4,16)13(15)12(11)15/h5-6,9-13,16H,7
<b>InchiKey:</b>	LMCRYOCEEDDKMQA-JCCYOPCHSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)C1C=CC(C)C23CCC(C)(O)C2C13
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	102.16	kJ/mol	Joback Method
hf	-270.96	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.242		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	644.46	K	Joback Method
tc	849.94	K	Joback Method
tf	390.77	K	Joback Method
vc	0.731	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.51	J/molxK	644.46	Joback Method
cpg	593.11	J/molxK	678.71	Joback Method
cpg	610.85	J/molxK	712.95	Joback Method
cpg	627.94	J/molxK	747.20	Joback Method
cpg	644.63	J/molxK	781.45	Joback Method

cpg	661.14	J/mol×K	815.69	Joback Method
cpg	677.70	J/mol×K	849.94	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=R600443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R600443&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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