

# cis-Bejarol

<b>Other names:</b>	erythro-cis-Bejarol (9-epi-5,9-Epoxynerolidol)
<b>Inchi:</b>	InChI=1S/C15H24O2/c1-6-15(5,16)10-14-9-12(4)8-13(17-14)7-11(2)3/h6-7,9,13-14,16H,
<b>InchiKey:</b>	NNCJOVBGLCRHAN-ZYOSVBKOSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	<chem>C=CC(C)(O)CC1C=C(C)CC(C=C(C)C)O1</chem>
<b>Mol. weight [g/mol]:</b>	236.35

## Physical Properties

Property code	Value	Unit	Source
gf	51.90	kJ/mol	Joback Method
hf	-332.76	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.383		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1559.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2060.00		NIST Webbook
tb	678.24	K	Joback Method
tc	878.18	K	Joback Method
tf	344.24	K	Joback Method
vc	0.784	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.07	J/molxK	678.24	Joback Method
cpg	619.22	J/molxK	711.56	Joback Method
cpg	635.33	J/molxK	744.89	Joback Method
cpg	650.47	J/molxK	778.21	Joback Method
cpg	664.70	J/molxK	811.53	Joback Method

cpg	678.08	J/mol×K	844.85	Joback Method
cpg	690.67	J/mol×K	878.18	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=R232778&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R232778&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>hvp:</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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