

# trans-(Z)-Bisabolene epoxide

<b>Inchi:</b>	InChI=1S/C15H24O/c1-11(2)5-10-14-15(4,16-14)13-8-6-12(3)7-9-13/h5-6,13-14H,7-10H
<b>InchiKey:</b>	PBNXUEQZNAEDOI-ZNMIVQPWSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)=CCC1OC1(C)C1CC=C(C)CC1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	153.30	kJ/mol	Joback Method
hf	-209.17	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	599.59	K	Joback Method
tc	819.43	K	Joback Method
tf	324.60	K	Joback Method
vc	0.750	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.36	J/molxK	599.59	Joback Method
cpg	556.81	J/molxK	636.23	Joback Method
cpg	576.95	J/molxK	672.87	Joback Method
cpg	595.97	J/molxK	709.51	Joback Method
cpg	614.03	J/molxK	746.15	Joback Method
cpg	631.29	J/molxK	782.79	Joback Method
cpg	647.92	J/molxK	819.43	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R609900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R609900&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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