

# Humulene epoxide III

**Inchi:** InChI=1S/C15H26O/c1-11-6-5-7-12(2)10-13-14(16-13)15(3,4)9-8-11/h8,12-14H,5-7,9-10  
**InchiKey:** XFCFMJBRKXYZKP-QGIRJVRWSA-N  
**Formula:** C15H26O  
**SMILES:** CC1=CCC(C)(C)C2OC2CC(C)CCC1  
**Mol. weight [g/mol]:** 222.37

## Physical Properties

Property code	Value	Unit	Source
gf	37.62	kJ/mol	Joback Method
hf	-355.42	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.326		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
tb	603.69	K	Joback Method
tc	832.68	K	Joback Method
tf	328.84	K	Joback Method
vc	0.745	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.42	J/molxK	603.69	Joback Method
cpg	587.62	J/molxK	641.85	Joback Method
cpg	611.32	J/molxK	680.02	Joback Method
cpg	633.65	J/molxK	718.18	Joback Method
cpg	654.76	J/molxK	756.35	Joback Method
cpg	674.76	J/molxK	794.51	Joback Method
cpg	693.79	J/molxK	832.68	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R602058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R602058&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>

# 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>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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