

# Spathylenol

<b>Other names:</b>	(+)-spathulenol
<b>Inchi:</b>	InChI=1S/C15H24O/c1-9-5-6-11-13(14(11,2)3)12-10(9)7-8-15(12,4)16/h10-13,16H,1,5-8
<b>InchiKey:</b>	FRMCCTDTYSRUBE-YZXOMZRCSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC2C(C3C1CCC3(C)O)C2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	115.62	kJ/mol	Joback Method
hf	-245.38	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1575.00		NIST Webbook
tb	649.17	K	Joback Method
tc	856.86	K	Joback Method
tf	415.17	K	Joback Method
vc	0.727	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.53	J/molxK	649.17	Joback Method
cpg	594.60	J/molxK	683.79	Joback Method
cpg	612.82	J/molxK	718.40	Joback Method
cpg	630.40	J/molxK	753.02	Joback Method

cpg	647.59	J/mol×K	787.63	Joback Method
cpg	664.58	J/mol×K	822.25	Joback Method
cpg	681.62	J/mol×K	856.86	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=R281488&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R281488&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>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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