

# Verrucarol

<b>Other names:</b>	Trichothec-9-ene-4,15-diol, 12,13-epoxy-, (4«beta»)- Trichothec-9-ene-4«beta»,15-diol, 12,13-epoxy- Spiro[2,5-methano-1-benzoxepin-10,2'-oxirane], trichothec-9-ene-4,15-diol deriv. (4«beta»)-12,13-Epoxytrichothec-9-ene-4,15-diol
<b>Inchi:</b>	InChI=1S/C15H22O4/c1-9-3-4-14(7-16)11(5-9)19-12-10(17)6-13(14,2)15(12)8-18-15/h5,
<b>InchiKey:</b>	NBRKAFIHDFEBCP-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O4
<b>SMILES:</b>	<chem>CC1=CC2OC3C(O)CC(C)(C2(CO)CC1)C31CO1</chem>
<b>Mol. weight [g/mol]:</b>	266.33
<b>CAS:</b>	2198-92-7

## Physical Properties

Property code	Value	Unit	Source
gf	-163.22	kJ/mol	Joback Method
hf	-591.16	kJ/mol	Joback Method
hfus	31.16	kJ/mol	Joback Method
hvap	88.24	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.013		Crippen Method
mcvol	197.950	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
tb	811.88	K	Joback Method
tc	1024.45	K	Joback Method
tf	574.81	K	Joback Method
vc	0.746	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.77	J/molxK	811.88	Joback Method
cpg	701.65	J/molxK	847.31	Joback Method
cpg	720.39	J/molxK	882.74	Joback Method

cpg	740.35	J/mol×K	918.17	Joback Method
cpg	761.88	J/mol×K	953.59	Joback Method
cpg	785.34	J/mol×K	989.02	Joback Method
cpg	811.07	J/mol×K	1024.45	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2198927&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2198927&amp;Units=SI</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>rinpola:</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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