

# Vanillyl epoxijaeschkeanadiol

<b>Inchi:</b>	InChI=1S/C23H32O6/c1-13(2)23(26)9-8-21(3)12-18-22(4,29-18)11-17(19(21)23)28-20(2)
<b>InchiKey:</b>	LUXHNMNHDPKHBY-UXZPXHOFSA-N
<b>Formula:</b>	C23H32O6
<b>SMILES:</b>	COc1cc(C(=O)OC2CC3(C)OC3CC3(C)CCC(O)(C(C)C)C23)ccc1O
<b>Mol. weight [g/mol]:</b>	404.50

## Physical Properties

Property code	Value	Unit	Source
gf	-354.91	kJ/mol	Joback Method
hf	-946.05	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	110.81	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.681		Crippen Method
mcvol	309.510	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2863.00		NIST Webbook
tb	1070.79	K	Joback Method
tc	1316.63	K	Joback Method
tf	772.17	K	Joback Method
vc	1.103	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.07	J/molxK	1070.79	Joback Method
cpg	1261.55	J/molxK	1111.76	Joback Method
cpg	1307.05	J/molxK	1152.74	Joback Method
cpg	1357.10	J/molxK	1193.71	Joback Method
cpg	1412.26	J/molxK	1234.69	Joback Method
cpg	1473.08	J/molxK	1275.66	Joback Method
cpg	1540.10	J/molxK	1316.63	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=R200310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R200310&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>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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