

# gentisin

<b>Inchi:</b>	InChI=1S/C14H14O5/c1-18-8-5-10(16)13-12(6-8)19-11-3-2-7(15)4-9(11)14(13)17/h2-6,9
<b>InchiKey:</b>	XOXYHGOIRWABTC-UHFFFAOYSA-N
<b>Formula:</b>	C14H14O5
<b>SMILES:</b>	<chem>COC1=CC2OC3C=CC(O)=CC3C(=O)C2C(O)=C1</chem>
<b>Mol. weight [g/mol]:</b>	262.26

## Physical Properties

Property code	Value	Unit	Source
gf	-315.36	kJ/mol	Joback Method
hf	-674.70	kJ/mol	Joback Method
hfus	37.57	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Joback Method
log10ws	-2.93		Aqueous Solubility Prediction Method
log10ws	-2.94		Estimated Solubility Method
logp	1.553		Crippen Method
mcvol	183.390	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	869.75	K	Joback Method
tc	1088.21	K	Joback Method
tf	539.65	K	Aqueous Solubility Prediction Method
vc	0.677	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.03	J/molxK	869.75	Joback Method
cpg	612.26	J/molxK	906.16	Joback Method
cpg	622.47	J/molxK	942.57	Joback Method
cpg	631.68	J/molxK	978.98	Joback Method
cpg	639.89	J/molxK	1015.39	Joback Method
cpg	647.14	J/molxK	1051.80	Joback Method
cpg	653.44	J/molxK	1088.21	Joback Method

# Sources

<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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