

# Amigdalin

<b>Other names:</b>	amygdalin
<b>Inchi:</b>	InChI=1S/C20H27NO11/c21-6-10(9-4-2-1-3-5-9)30-20-18(28)16(26)14(24)12(32-20)8-29
<b>InchiKey:</b>	XUCIJNAGGSZNQT-UHFFFAOYSA-N
<b>Formula:</b>	C20H27NO11
<b>SMILES:</b>	<chem>N#CC(OC1OC(COC2OC(CO)C(O)C(O)C2O)C(O)C(O)C1O)c1ccccc1</chem>
<b>Mol. weight [g/mol]:</b>	457.43

## Physical Properties

Property code	Value	Unit	Source
gf	-992.09	kJ/mol	Joback Method
hf	-1708.13	kJ/mol	Joback Method
hfus	78.77	kJ/mol	Joback Method
hvap	201.46	kJ/mol	Joback Method
log10ws	-0.77		Estimated Solubility Method
log10ws	-0.77		Aqueous Solubility Prediction Method
logp	-3.108		Crippen Method
mcvol	313.130	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	1531.06	K	Joback Method
tc	2253.10	K	Joback Method
tf	497.65	K	Aqueous Solubility Prediction Method
vc	1.137	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.35	J/molxK	1531.06	Joback Method
cpg	1017.75	J/molxK	1651.40	Joback Method
cpg	917.68	J/molxK	1771.74	Joback Method
cpg	792.93	J/molxK	1892.08	Joback Method
cpg	643.31	J/molxK	2012.42	Joback Method
cpg	468.60	J/molxK	2132.76	Joback Method

## Sources

<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/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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>

## 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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