

# 5-Vanillylidene barbituric acid

<b>Inchi:</b>	InChI=1S/C12H10N2O5/c1-19-9-5-6(2-3-8(9)15)4-7-10(16)13-12(18)14-11(7)17/h2-5,15
<b>InchiKey:</b>	HOHWOUABYDGBN-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N2O5
<b>SMILES:</b>	COc1cc(C=C2C(O)=NC(=O)N=C2O)ccc1O
<b>Mol. weight [g/mol]:</b>	262.22
<b>CAS:</b>	40367-32-6

## Physical Properties

Property code	Value	Unit	Source
gf	-151.07	kJ/mol	Joback Method
hf	-432.39	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	114.13	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.831		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
pc	5160.85	kPa	Joback Method
tb	1007.38	K	Joback Method
tc	1252.10	K	Joback Method
tf	779.37	K	Joback Method
vc	0.616	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.59	J/molxK	1007.38	Joback Method
cpg	587.10	J/molxK	1048.17	Joback Method
cpg	592.36	J/molxK	1088.95	Joback Method
cpg	596.38	J/molxK	1129.74	Joback Method
cpg	599.15	J/molxK	1170.53	Joback Method
cpg	600.66	J/molxK	1211.31	Joback Method
cpg	600.91	J/molxK	1252.10	Joback Method

# Sources

<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>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=C40367326&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40367326&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>mccvol:</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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