

# Phenytoin, M(HO-), AC

<b>Inchi:</b>	InChI=1S/C17H14N2O4/c1-11(20)23-14-9-7-13(8-10-14)17(12-5-3-2-4-6-12)15(21)18-16
<b>InchiKey:</b>	OHIPXMKWHVEHCR-UHFFFAOYSA-N
<b>Formula:</b>	C17H14N2O4
<b>SMILES:</b>	CC(=O)Oc1ccc(C2(c3ccccc3)NC(=O)NC2=O)cc1
<b>Mol. weight [g/mol]:</b>	310.30

## Physical Properties

Property code	Value	Unit	Source
gf	34.83	kJ/mol	Joback Method
hf	-301.48	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	88.92	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	1.695		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	971.25	K	Joback Method
tc	1256.88	K	Joback Method
tf	800.17	K	Joback Method
vc	0.823	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.38	J/molxK	971.25	Joback Method
cpg	721.33	J/molxK	1018.85	Joback Method
cpg	736.33	J/molxK	1066.46	Joback Method
cpg	750.52	J/molxK	1114.06	Joback Method
cpg	764.01	J/molxK	1161.67	Joback Method
cpg	776.95	J/molxK	1209.27	Joback Method
cpg	789.45	J/molxK	1256.88	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=R254956&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R254956&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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