

# 7,9-diazaspiro[4.5]decane-6,8,10-trione

<b>Other names:</b>	cyclopentyl-5-spirobarbituric acid
<b>Inchi:</b>	InChI=1S/C8H10N2O3/c11-5-8(3-1-2-4-8)6(12)10-7(13)9-5/h1-4H2,(H2,9,10,11,12,13)
<b>InchiKey:</b>	HYPRUQJUBWRVEM-UHFFFAOYSA-N
<b>Formula:</b>	C8H10N2O3
<b>SMILES:</b>	O=C1NC(=O)C2(CCCC2)C(=O)N1
<b>Mol. weight [g/mol]:</b>	182.18

## Physical Properties

Property code	Value	Unit	Source
gf	-100.55	kJ/mol	Joback Method
hf	-389.39	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-2.35		Aqueous Solubility Prediction Method
log10ws	-2.35		Estimated Solubility Method
log10ws	-2.35		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.087		Crippen Method
mcvol	126.530	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
tb	718.47	K	Joback Method
tc	1012.20	K	Joback Method
tf	644.58	K	Joback Method
vc	0.460	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.92	J/mol×K	718.47	Joback Method
cpg	388.44	J/mol×K	767.42	Joback Method
cpg	404.97	J/mol×K	816.38	Joback Method
cpg	420.56	J/mol×K	865.33	Joback Method

cpg	435.29	J/mol×K	914.29	Joback Method
cpg	449.20	J/mol×K	963.24	Joback Method
cpg	462.36	J/mol×K	1012.20	Joback Method

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:** [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)

**Aqueous and cosolvent solubility data** <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

**for drug-like organic compounds:**

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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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