

# 1,3-Diazaspiro(4.4)nonane-2,4-dione

<b>Inchi:</b>	InChI=1S/C7H10N2O2/c10-5-7(3-1-2-4-7)9-6(11)8-5/h1-4H2,(H2,8,9,10,11)
<b>InchiKey:</b>	JTTFXYHJDZZDQK-UHFFFAOYSA-N
<b>Formula:</b>	C7H10N2O2
<b>SMILES:</b>	O=C1NC(=O)C2(CCCC2)N1
<b>Mol. weight [g/mol]:</b>	154.17
<b>CAS:</b>	699-51-4

## Physical Properties

Property code	Value	Unit	Source
gf	25.72	kJ/mol	Joback Method
hf	-224.89	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	52.69	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.139		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	623.50	K	Joback Method
tc	903.07	K	Joback Method
tf	568.61	K	Joback Method
vc	0.405	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.18	J/molxK	623.50	Joback Method
cpg	311.17	J/molxK	670.09	Joback Method
cpg	326.28	J/molxK	716.69	Joback Method
cpg	340.63	J/molxK	763.28	Joback Method
cpg	354.36	J/molxK	809.88	Joback Method
cpg	367.59	J/molxK	856.47	Joback Method
cpg	380.46	J/molxK	903.07	Joback Method

# Sources

<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=C699514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C699514&amp;Units=SI</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>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>

# 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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