

# 5-Nitro-1-anthraquinonesulfonic acid

<b>Other names:</b>	9,10-dihydro-5-nitro-9,10-dioxoanthracenesulphonic acid
<b>Inchi:</b>	InChI=1S/C14H7NO7S/c16-13-8-4-2-6-10(23(20,21)22)12(8)14(17)7-3-1-5-9(11(7)13)15
<b>InchiKey:</b>	JFORTLRWSWJGGI-UHFFFAOYSA-N
<b>Formula:</b>	C14H7NO7S
<b>SMILES:</b>	O=C1c2cccc(S(=O)(=O)O)c2C(=O)c2cccc([N+](=O)[O-])c21
<b>Mol. weight [g/mol]:</b>	333.27
<b>CAS:</b>	82-50-8

## Physical Properties

Property code	Value	Unit	Source
gf	-481.13	kJ/mol	Joback Method
hf	-697.55	kJ/mol	Joback Method
hfus	43.55	kJ/mol	Joback Method
hvap	114.41	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	1.617		Crippen Method
mcvol	204.260	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	1027.58	K	Joback Method
tc	1285.64	K	Joback Method
tf	755.59	K	Joback Method
vc	0.810	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.93	J/molxK	1027.58	Joback Method
cpg	604.75	J/molxK	1070.59	Joback Method
cpg	608.10	J/molxK	1113.60	Joback Method
cpg	610.00	J/molxK	1156.61	Joback Method
cpg	610.44	J/molxK	1199.62	Joback Method
cpg	609.42	J/molxK	1242.63	Joback Method
cpg	606.96	J/molxK	1285.64	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C82508&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82508&amp;Units=SI</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</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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