

# 1,4-diaminoanthraquinone

<b>Inchi:</b>	InChI=1S/C14H10N2O2/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-6H,1
<b>InchiKey:</b>	FBMQNRKSAWNXBT-UHFFFAOYSA-N
<b>Formula:</b>	C14H10N2O2
<b>SMILES:</b>	<chem>Nc1ccc(N)c2c1C(=O)c1cccc1C2=O</chem>
<b>Mol. weight [g/mol]:</b>	238.25

## Physical Properties

Property code	Value	Unit	Source
gf	221.58	kJ/mol	Joback Method
hf	-13.63	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	83.78	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.626		Crippen Method
mvol	172.840	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	880.84	K	Joback Method
tc	1161.76	K	Joback Method
tf	516.27	K	Solubility of C.I. Disperse Violet 1 in Supercritical Carbon Dioxide with or without Cosolvent
vc	0.641	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.63	J/molxK	880.84	Joback Method
cpg	518.91	J/molxK	927.66	Joback Method
cpg	528.94	J/molxK	974.48	Joback Method
cpg	537.75	J/molxK	1021.30	Joback Method
cpg	545.39	J/molxK	1068.12	Joback Method
cpg	551.89	J/molxK	1114.94	Joback Method
cpg	557.29	J/molxK	1161.76	Joback Method

# Sources

<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>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Solubility of C.I. Disperse Violet 1 in Supercritical Carbon Dioxide with or without Cosolvent:</b>	<a href="https://www.doi.org/10.1021/je8003673">https://www.doi.org/10.1021/je8003673</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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