

# 2-Acetylamino-3-amino-1,4-naphthoquinone

<b>Inchi:</b>	InChI=1S/C12H10N2O3/c1-6(15)14-10-9(13)11(16)7-4-2-3-5-8(7)12(10)17/h2-5H,13H2,1
<b>InchiKey:</b>	IZJNNHJVNPVRHJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N2O3
<b>SMILES:</b>	CC(=O)NC1=C(N)C(=O)c2ccccc2C1=O
<b>Mol. weight [g/mol]:</b>	230.22
<b>CAS:</b>	13755-96-9

## Physical Properties

Property code	Value	Unit	Source
gf	1.74	kJ/mol	Joback Method
hf	-244.85	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	79.57	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	0.372		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	842.63	K	Joback Method
tc	1102.92	K	Joback Method
tf	630.69	K	Joback Method
vc	0.620	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.45	J/molxK	842.63	Joback Method
cpg	491.52	J/molxK	886.01	Joback Method
cpg	501.30	J/molxK	929.39	Joback Method
cpg	509.80	J/molxK	972.78	Joback Method
cpg	517.00	J/molxK	1016.16	Joback Method
cpg	522.87	J/molxK	1059.54	Joback Method
cpg	527.41	J/molxK	1102.92	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=C13755969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13755969&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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