

# 1-aminonaphthalene-2-sulfonic acid

<b>Inchi:</b>	InChI=1S/C10H9NO3S/c11-10-8-4-2-1-3-7(8)5-6-9(10)15(12,13)14/h1-6H,11H2,(H,12,13)
<b>InchiKey:</b>	ONZWNZGVZFLMNZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H9NO3S
<b>SMILES:</b>	<chem>Nc1c(S(=O)(=O)O)ccc2ccccc12</chem>
<b>Mol. weight [g/mol]:</b>	223.25

## Physical Properties

Property code	Value	Unit	Source
gf	-305.79	kJ/mol	Joback Method
hf	-416.86	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-1.66		Aqueous Solubility Prediction Method
logp	1.669		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	696.31	K	Joback Method
tc	915.54	K	Joback Method
tf	469.26	K	Joback Method
vc	0.584	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.65	J/mol×K	696.31	Joback Method
cpg	394.35	J/mol×K	732.85	Joback Method
cpg	403.26	J/mol×K	769.39	Joback Method
cpg	411.43	J/mol×K	805.93	Joback Method
cpg	418.88	J/mol×K	842.47	Joback Method
cpg	425.66	J/mol×K	879.00	Joback Method
cpg	431.79	J/mol×K	915.54	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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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