

# 4-dimethylaminodiazonylbenzoic acid

<b>Inchi:</b>	InChI=1S/C9H11N3O2/c1-12(2)11-10-8-5-3-7(4-6-8)9(13)14/h3-6H,1-2H3,(H,13,14)
<b>InchiKey:</b>	GUAZPUYTLMUTMA-UHFFFAOYSA-N
<b>Formula:</b>	C9H11N3O2
<b>SMILES:</b>	CN(C)N=Nc1ccc(C(=O)O)cc1
<b>Mol. weight [g/mol]:</b>	193.21

## Physical Properties

Property code	Value	Unit	Source
hf	-154.09	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-0.80		Aqueous Solubility Prediction Method
logp	1.945		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	744.67	K	Joback Method
tc	965.25	K	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>hf:</b>	Enthalpy of formation 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

**pc:** Critical Pressure  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature

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