

4-dimethylaminodiazonylbenzoic acid

Inchi:	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)
InchiKey:	GUAZPUYTLMUTMA-UHFFFAOYSA-N
Formula:	C9H11N3O2
SMILES:	CN(C)N=Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	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

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>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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

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