4-dimethylaminodiazenylbenzoic 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/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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