

nicotinamide

Inchi: InChI=1S/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)
InchiKey: DFPAKSUCGFBDDE-UHFFFAOYSA-N
Formula: C6H6N2O
SMILES: NC(=O)c1cccnc1
Mol. weight [g/mol]: 122.13

Physical Properties

Property code	Value	Unit	Source
log10ws	0.61		Aqueous Solubility Prediction Method
log10ws	0.61		Estimated Solubility Method
logp	0.181		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
tf	403.05	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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