# nicotinamide

**Inchi:** InChI=1S/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)
**InchiKey:** DFPAKSUCGFBDDF-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/ci990307l
**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
**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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