

# Niridazole

**Inchi:** InChI=1S/C6H6N4O3S/c11-5-7-1-2-9(5)6-8-3-4(14-6)10(12)13/h3H,1-2H2,(H,7,11)  
**InchiKey:** RDXLYGJSWZYTFJ-UHFFFAOYSA-N  
**Formula:** C6H6N4O3S  
**SMILES:** O=C1NCCN1c1ncc([N+](=O)[O-])s1  
**Mol. weight [g/mol]:** 214.21

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -3.22   |        | Aqueous Solubility Prediction Method |
| log10ws       | -3.22   |        | Estimated Solubility Method          |
| logp          | 0.581   |        | Crippen Method                       |
| mcvol         | 130.360 | ml/mol | McGowan Method                       |

## Sources

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

**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](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

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