

# ISOQUINOLINE 1,2,3,4-TETRAHYDRO-2-NITRO-

**Other names:** 1-nitro-3,4-benzo-1-azacyclohexane  
**Inchi:** InChI=1S/C9H10N2O2/c12-11(13)10-6-5-8-3-1-2-4-9(8)7-10/h1-4H,5-7H2  
**InchiKey:** DEIUMGGCQWPHNC-UHFFFAOYSA-N  
**Formula:** C9H10N2O2  
**SMILES:** O=[N+](O-)[N]1CCc2ccccc2C1  
**Mol. weight [g/mol]:** 178.19

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 1.236   |        | Crippen Method |
| mcvol         | 130.450 | ml/mol | McGowan Method |

## Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10308722&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/119-150-3/ISOQUINOLINE-1-2-3-4-TETRAHYDRO-2-NITRO.pdf>

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