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-])N1CCc2ccccc2C1
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

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume