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
CAS:	10308-72-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.236		Crippen Method
mcvol	130.450	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10308722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume