1,4-Ethanoquinoxaline, 2,3-dihydro-

Other names: Benzo[b]-1,4-diazabicyclo[2.2.2]octane
Inchi: InChI=1S/C10H12N2/c1-2-4-10-9(3-1)11-5-7-12(10)8-6-11/h1-4H,5-8H2
InchiKey: OGEXWIXITOCNRZ-UHFFFAOYSA-N
Formula: C10H12N2
SMILES: c1ccc2c(c1)N1CCN2CC1
Mol. weight [g/mol]: 160.22
CAS: 7140-45-6

Physical Properties

Property code	Value	Unit	Source
ie	7.92	eV	NIST Webbook
log10ws	-1.08		Crippen Method
logp	1.327		Crippen Method
mcvol	126.240	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=C7140456&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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