2H-1,4-Ethanoquinoline, 3,4-dihydro-

Other names:	Benzoquinuclidine
	3,4-Dihydro-2H-1,4-ethanoquinoline
	1,4-Dihydro-1,4-Ethanoquinoline
Inchi:	InChI=1S/C11H13N/c1-2-4-11-10(3-1)9-5-7-12(11)8-6-9/h1-4,9H,5-8H2
InchiKey:	RNFRFPSSWGWDKI-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	c1ccc2c(c1)C1CCN2CC1
Mol. weight [g/mol]:	159.23
CAS:	4363-25-1

Physical Properties

Property code	Value	Unit	Source
affp	979.80	kJ/mol	NIST Webbook
basg	948.80	kJ/mol	NIST Webbook
ie	7.85 ± 0.02	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.384		Crippen Method
mcvol	130.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4363251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume