2-Ethoxyquinoline

Inchi: InChI=1S/C11H11NO/c1-2-13-11-8-7-9-5-3-4-6-10(9)12-11/h3-8H,2H2,1H3
InchiKey: AZJQQNWSSLCLJN-UHFFFAOYSA-N
Formula: C11H11NO
SMILES: CCOc1ccc2ccccc2n1
Mol. weight [g/mol]: 173.21
CAS: 46185-83-5

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	2.633		Crippen Method
mcvol	138.480	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C46185835&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

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