Benzo[f]isoquinoline

Other names: 5,6-Benzoisoquinoline
Inchi: InChI=1S/C13H9N/c1-2-4-12-10(3-1)5-6-11-9-14-8-7-13(11)12/h1-9H
InchiKey: JQXCGCPMGZBMLE-UHFFFAOYSA-N
Formula: C13H9N
SMILES: c1ccc2c(c1)ccc1cnccc12
Mol. weight [g/mol]: 179.22
CAS: 229-67-4

Physical Properties

Property code	Value	Unit	Source
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-4.85		Crippen Method
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C229674&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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