Benzo[f]quinoxaline

Inchi: InChI=1S/C12H8N2/c1-2-4-10-9(3-1)5-6-11-12(10)14-8-7-13-11/h1-8H
InchiKey: YUFRAQHYKKPYLH-UHFFFAOYSA-N
Formula: C12H8N2
SMILES: c1ccc2c(c1)ccc1nccnc12
Mol. weight [g/mol]: 180.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Aqueous Solubility Prediction Method
logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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