

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:	YUFRAQHKKPYLH-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/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/100-766-0/Benzo-f-quinoxaline.pdf>

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