2-Phenyl-3,1-benzoxazin-4-one

Inchi: InChI=1S/C14H9NO2/c16-13-11-8-4-5-9-12(11)17-14(15-13)10-6-2-1-3-7-10/h1-9H
InchiKey: GWDYJKXSUSPLEA-UHFFFAOYSA-N
Formula: C14H9NO2
SMILES: O=c1nc(-c2ccccc2)oc2ccccc12
Mol. weight [g/mol]: 223.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Aqueous Solubility Prediction Method
logp	2.855		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
tf	396.65	K	Aqueous Solubility Prediction Method

Sources

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.