2,3-Dihydro-2-phenyl-1h-1,3,2-benzodiazaborole

Inchi: InChI=1S/C12H11BN2/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9,14-15H
InchiKey: BPFCMNQMCJTFBC-UHFFFAOYSA-N
Formula: C12H11BN2
SMILES: c1ccc(B2Nc3ccccc3N2)cc1
Mol. weight [g/mol]: 194.04
CAS: 2479-64-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	1.919		Crippen Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2479643&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient