6-Phenylisoquinoline

Other names: Isoquinoline, 6-phenyl-
Inchi: InChI=1S/C15H11N/c1-2-4-12(5-3-1)13-6-7-15-11-16-9-8-14(15)10-13/h1-11H
InchiKey: CNTILWPLENFTMZ-UHFFFAOYSA-N
Formula: C15H11N
SMILES: c1ccc(-c2ccc3cnccc3c2)cc1
Mol. weight [g/mol]: 205.25
CAS: 70125-61-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	3.902		Crippen Method
mcvol	165.210	ml/mol	McGowan Method
rinpol	2029.80		NIST Webbook
rinpol	2029.80		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C70125610&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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