

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:	<chem>c1ccc(-c2ccc3cnccc3c2)cc1</chem>
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
rinsol	2029.80		NIST Webbook
rinsol	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
rinsol:	Non-polar retention indices

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