Isoquinoline, 1-phenyl-

Other names:	1-Phenylisoquinoline
Inchi:	InChI=1S/C15H11N/c1-2-7-13(8-3-1)15-14-9-5-4-6-12(14)10-11-16-15/h1-11H
InchiKey:	LPCWDYWZIWDTCV-UHFFFAOYSA-N
Formula:	C15H11N
SMILES:	c1ccc(-c2nccc3ccccc23)cc1
Mol. weight [g/mol]:	205.25
CAS:	3297-72-1

Physical Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	571.20	K	97.20	NIST Webbook
tbrp	403.20	K	0.10	NIST Webbook

Sources

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=C3297721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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