

Imolamine

Inchi:	InChI=1S/C14H20N4O/c1-3-17(4-2)10-11-18-13(16-19-14(18)15)12-8-6-5-7-9-12/h5-9,1
InchiKey:	MGSPDRWOUCPKNZ-UHFFFAOYSA-N
Formula:	C14H20N4O
SMILES:	CCN(CC)CCn1c(-c2ccccc2)noc1=N
Mol. weight [g/mol]:	260.33
CAS:	318-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.07		Crippen Method
logp	1.964		Crippen Method
mcvol	210.690	ml/mol	McGowan Method
rmpol	2136.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C318230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
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
rmpol:	Non-polar retention indices

Latest version available from:

<https://www.chemed.com/cid/34-972-5/Imolamine.pdf>

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