3-Isoquinolinecarbonitrile

Inchi: InChI=1S/C10H6N2/c11-6-10-5-8-3-1-2-4-9(8)7-12-10/h1-5,7H
InchiKey: GXXBVBVNGMCFIU-UHFFFAOYSA-N
Formula: C10H6N2
SMILES: N#Cc1cc2ccccc2cn1
Mol. weight [g/mol]: 154.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.106		Crippen Method
mcvol	119.900	ml/mol	McGowan Method
rinpol	1560.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R503738&Units=SI
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

Legend

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