4-(2-Methylpropyl)isoquinoline

Inchi: InChI=1S/C13H15N/c1-10(2)7-12-9-14-8-11-5-3-4-6-13(11)12/h3-6,8-10H,7H2,1-2H3
InchiKey: FOLWHSQHXGHOHN-UHFFFAOYSA-N
Formula: C13H15N
SMILES: CC(C)Cc1cncc2ccccc12
Mol. weight [g/mol]: 185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.433		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R545470&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.