

4-(1-Methylpropyl)isoquinoline

Inchi: InChI=1S/C13H15N/c1-3-10(2)13-9-14-8-11-6-4-5-7-12(11)13/h4-10H,3H2,1-2H3
InchiKey: VEYAUUGPGBVYDP-UHFFFAOYSA-N
Formula: C13H15N
SMILES: CCC(C)c1cncc2ccccc12
Mol. weight [g/mol]: 185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.748		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1667.00		NIST Webbook
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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=R545465&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/54-311-6/4-1-Methylpropyl-isoquinoline.pdf>

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