

2-(3-Phenylpropyl)pyridine

Inchi: InChI=1S/C14H15N/c1-2-7-13(8-3-1)9-6-11-14-10-4-5-12-15-14/h1-5,7-8,10,12H,6,9,11H
InchiKey: JJJPNTQYUJPGWQ-UHFFFAOYSA-N
Formula: C14H15N
SMILES: c1ccc(CCCc2cccn2)cc1
Mol. weight [g/mol]: 197.28
CAS: 2110-18-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	3.257		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
rinpola	1660.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C2110181&Units=SI>

Legend

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

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