

4-(3-Phenoxypropyl)pyridine

Inchi: InChI=1S/C14H15NO/c1-2-6-14(7-3-1)16-12-4-5-13-8-10-15-11-9-13/h1-3,6-11H,4-5,12H
InchiKey: TYMHXGLDRUMFJW-UHFFFAOYSA-N
Formula: C14H15NO
SMILES: c1ccc(OCCCc2ccncc2)cc1
Mol. weight [g/mol]: 213.28

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.81 | | Crippen Method |
| logp | 3.093 | | Crippen Method |
| mcvol | 176.450 | ml/mol | McGowan Method |
| rinsol | 1887.00 | | 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=R545490&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/28-962-3/4-3-Phenoxypropyl-pyridine.pdf>

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