

Pyrazine, 2-pentyl-3-phenylthio

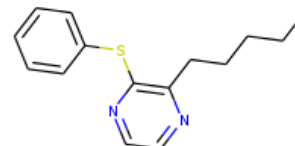
InChI: InChI=1S/C15H18N2S/c1-2-3-5-10-14-15(17-12-11-16-14)18-13-8-6-4-7-9-13/h4,6-9,11-12H,2-3,5,10H2,1H3

InChI Key: FOIHOLTYNMLOGQ-UHFFFAOYSA-N

Formula: C15H18N2S

SMILES: CCCCCc1nccnc1Sc1ccccc1

Molecular Weight: 258.38



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 4.361 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H18N2S/c1-2-3-5-10-14-15\(17-12-11-16-14\)18-13-8-6-4-7-9-13/h4,6-9,11-12H,2-3,5,10H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H18N2S/c1-2-3-5-10-14-15(17-12-11-16-14)18-13-8-6-4-7-9-13/h4,6-9,11-12H,2-3,5,10H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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