

1-(2-phenylethyl)-2-formylpyrrol

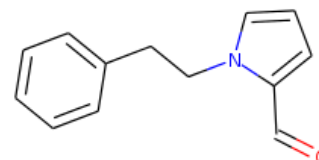
InChI: InChI=1S/C13H13NO/c15-11-13-7-4-9-14(13)10-8-12-5-2-1-3-6-12/h1-7,9,11H,8,10H2

InChI Key: ITWVWJWDKXWQFS-UHFFFAOYSA-N

Formula: C13H13NO

SMILES: O=Cc1cccn1CCc1ccccc1

Molecular Weight: 199.25



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.54		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H13NO/c15-11-13-7-4-9-14\(13\)10-8-12-5-2-1-3-6-12/h1-7,9,11H,8,10H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H13NO/c15-11-13-7-4-9-14(13)10-8-12-5-2-1-3-6-12/h1-7,9,11H,8,10H2)

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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