

Alpha,alpha-difluorophenacyl pyrazine

InChI: InChI=1S/C12H8F2N2O/c13-12(14,10-8-15-6-7-16-10)11(17)9-4-2-1-3-5-9/h1-8H

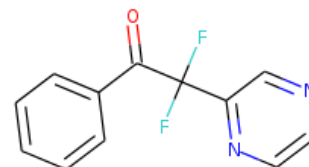
InChI Key: HFQPREQQQACYNB-UHFFFAOYSA-N

Formula: C12H8F2N2O

SMILES: O=C(c1ccccc1)C(F)(F)c1cnccn1

Molecular Weight: 234.20

CAS: 116403-02-2



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 2.45 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8F2N2O/c13-12\(14,10-8-15-6-7-16-10\)11\(17\)9-4-2-1-3-5-9/h1-8H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8F2N2O/c13-12(14,10-8-15-6-7-16-10)11(17)9-4-2-1-3-5-9/h1-8H)

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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