

9H-purine, 9-benzyl-6-methyl-

InChI: InChI=1S/C13H12N4/c1-10-12-13(15-8-14-10)17(9-16-12)7-11-5-3-2-4-6-11/h2-6,8-9H,7H2,1H3

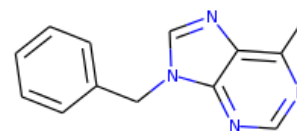
InChI Key: QKVCUXBATHLQSL-UHFFFAOYSA-N

Formula: C13H12N4

SMILES: Cc1ncnc2c1ncn2Cc1ccccc1

Molecular Weight: 224.26

CAS: 160516-13-2



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 2.183 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H12N4/c1-10-12-13\(15-8-14-10\)17\(9-16-12\)7-11-5-3-2-4-6-11/h2-6,8-9H,7H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H12N4/c1-10-12-13(15-8-14-10)17(9-16-12)7-11-5-3-2-4-6-11/h2-6,8-9H,7H2,1H3)

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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