

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

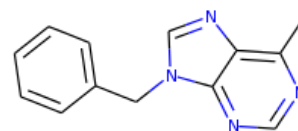
InChI Key: QKVCUXBATHLQSL-UHFFFAOYSA-N

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 .

Latest version available from:

<https://www.cheméo.com/cid/10-284-5/9H-purine%2C%209-benzyl-6-methyl->

Generated by Cheméo on Sun, 18 Nov 2018 05:40:14 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.