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

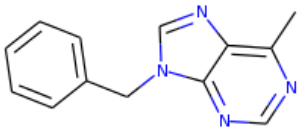
InChI Key: QKVCUXBATHLQSL-UHFFFAOYSA-N

Formula: C13H12N4

SMILES: Cc1ncnc2c1ncn2Cc1ccccc1

Molecular Weight: 224.26

CAS: 160516-13-2



Physical Properties

Property	Value	Unit	Source
*log*P$_{oct/wat}$	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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .