9H-purine, 2,6-diamino-9-benzyl-

Inchi: InChI=1S/C12H12N6/c13-10-9-11(17-12(14)16-10)18(7-15-9)6-8-4-2-1-3-5-8/h1-5,7H,6H
InchiKey: DRGHOMRXJSSSBT-UHFFFAOYSA-N
Formula: C12H12N6
SMILES: N=c1nc2c(ncn2Cc2ccccc2)c(N)[nH]1
Mol. weight [g/mol]: 240.26
CAS: 7674-36-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Crippen Method
logp	0.387		Crippen Method
mcvol	177.140	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7674364&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume