

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:	<chem>N=c1nc2c(ncn2Cc2ccccc2)c(N)[nH]1</chem>
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

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