

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,7
InchiKey:	QKVCUXBATHLQSL-UHFFFAOYSA-N
Formula:	C13H12N4
SMILES:	Cc1ncnc2c1ncn2Cc1ccccc1
Mol. weight [g/mol]:	224.26
CAS:	160516-13-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	2.183		Crippen Method
mcvol	171.270	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C160516132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/10-284-5/9H-purine-9-benzyl-6-methyl.pdf>

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