

9H-purin-6(1h)-one, 9-benzyl-2-dimethylamino-

Inchi:	InChI=1S/C14H15N5O/c1-18(2)14-16-12-11(13(20)17-14)15-9-19(12)8-10-6-4-3-5-7-10/
InchiKey:	UUEQDDWCTVFZEV-UHFFFAOYSA-N
Formula:	C14H15N5O
SMILES:	CN(C)c1nc2c(ncn2Cc2ccccc2)c(=O)[nH]1
Mol. weight [g/mol]:	269.30
CAS:	7461-80-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	0.752		Crippen Method
mcvol	201.210	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7461805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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