

6-Benzylaminopurine, N,N'-dimethyl-

Inchi:	InChI=1S/C14H15N5/c1-18(8-11-6-4-3-5-7-11)14-12-13(15-9-16-14)17-10-19(12)2/h3-7,
InchiKey:	BQEXIWGJHQRULH-UHFFFAOYSA-N
Formula:	C14H15N5
SMILES:	CN(Cc1ccccc1)c1ncnc2ncn(C)c12
Mol. weight [g/mol]:	253.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	2.000		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
rinpola	2413.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/13-742-3/6-Benzylaminopurine-N-N-dimethyl.pdf>

Generated by Cheméo on 2024-04-27 09:05:50.980406691 +0000 UTC m=+16497999.900984003.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.