

7H-Purine, 7-benzyl-2,6-dichloro-

Other names:	9H-Purine, 9-benzyl-2, 6-dichloro-
Inchi:	InChI=1S/C12H8Cl2N4/c13-10-9-11(17-12(14)16-10)18(7-15-9)6-8-4-2-1-3-5-8/h1-5,7H,
InchiKey:	CUYCHULDTCBWLI-UHFFFAOYSA-N
Formula:	C12H8Cl2N4
SMILES:	Clc1nc(Cl)c2ncn(Cc3ccccc3)c2n1
Mol. weight [g/mol]:	279.12
CAS:	79064-26-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	3.181		Crippen Method
mcvol	181.660	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79064269&Units=SI

Legend

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

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