

9H-purine, 9-benzyl-6,8-dichloro-

Inchi:	InChI=1S/C12H8Cl2N4/c13-10-9-11(16-7-15-10)18(12(14)17-9)6-8-4-2-1-3-5-8/h1-5,7H,
InchiKey:	UJISOIMQMJRAFD-UHFFFAOYSA-N
Formula:	C12H8Cl2N4
SMILES:	Clc1ncnc2c1nc(Cl)n2Cc1ccccc1
Mol. weight [g/mol]:	279.12
CAS:	91395-18-5

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91395185&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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