

Hypoxanthine, 9-benzyl-2-chloro-

Inchi:	InChI=1S/C12H9ClN4O/c13-12-15-10-9(11(18)16-12)14-7-17(10)6-8-4-2-1-3-5-8/h1-5,7H
InchiKey:	LQIHZDQWYQABII-UHFFFAOYSA-N
Formula:	C12H9ClN4O
SMILES:	O=c1[nH]c(Cl)nc2c1ncn2Cc1ccccc1
Mol. weight [g/mol]:	260.68
CAS:	95194-86-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	1.339		Crippen Method
mcvol	175.290	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=C95194868&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/122-000-5/Hypoxanthine-9-benzyl-2-chloro.pdf>

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