

Purin-8(9h)-one, 9-benzyl-6-chloro-

Inchi:	InChI=1S/C12H9ClN4O/c13-10-9-11(15-7-14-10)17(12(18)16-9)6-8-4-2-1-3-5-8/h1-5,7H,
InchiKey:	URBCXJFWJJSOASL-UHFFFAOYSA-N
Formula:	C12H9ClN4O
SMILES:	O=c1[nH]c2c(Cl)ncnc2n1Cc1ccccc1
Mol. weight [g/mol]:	260.68
CAS:	21266-37-5

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21266375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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