

9H-purine-6(1h)-thione, 2-amino-9-benzyl-

Inchi:	InChI=1S/C12H11N5S/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:	VWIJTDSXILJLSY-UHFFFAOYSA-N
Formula:	C12H11N5S
SMILES:	<chem>N=c1nc(S)c2ncn(Cc3ccccc3)c2[nH]1</chem>
Mol. weight [g/mol]:	257.31
CAS:	92723-90-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	1.094		Crippen Method
mcvol	183.510	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=C92723905&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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