7H-tetrazolo[5,1-i]purine, 7-benzyl-

Inchi:	InChI=1S/C12H9N7/c1-2-4-9(5-3-1)6-18-7-13-10-11(18)14-8-19-12(10)15-16-17-19/h1-5
InchiKey:	HOHUVIRJDOLSQB-UHFFFAOYSA-N
Formula:	C12H9N7
SMILES:	c1ccc(Cn2cnc3c2ncn2nnnc32)cc1
Mol. weight [g/mol]:	251.25
CAS:	10553-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	0.917		Crippen Method
mcvol	171.960	ml/mol	McGowan Method

Sources

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=C10553443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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