

As-triazino[5,6-b]indole, 3-(3'-hydroxypropylamino)-5-methyl-

Inchi:	InChI=1S/C13H15N5O/c1-18-10-6-3-2-5-9(10)11-12(18)15-13(17-16-11)14-7-4-8-19/h2-3
InchiKey:	HAFUDIVSEQDBAY-UHFFFAOYSA-N
Formula:	C13H15N5O
SMILES:	Cn1c2ccccc2c2nnc(=NCCCO)[nH]c21
Mol. weight [g/mol]:	257.29
CAS:	4046-86-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	0.251		Crippen Method
mcvol	191.420	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=C4046860&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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