

3-Phenylazopyridine-2,6-diamine, N2-acetyl-

Other names:	N-(6-amino-5-((E)-phenyldiazenyl)pyridin-2-yl)acetamide
Inchi:	InChI=1S/C13H13N5O/c1-9(19)15-12-8-7-11(13(14)16-12)18-17-10-5-3-2-4-6-10/h2-8H,
InchiKey:	YBAFUGALWDQLSE-UHFFFAOYSA-N
Formula:	C13H13N5O
SMILES:	CC(=O)Nc1ccc(N=Nc2ccccc2)c(N)n1
Mol. weight [g/mol]:	255.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	3.038		Crippen Method
mcvol	193.680	ml/mol	McGowan Method
rinpola	2656.00		NIST Webbook

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=U373244&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
rinpola:	Non-polar retention indices

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