

As-triazine, 3-amino-5,6-di-2-pyridyl-

Inchi:	InChI=1S/C13H10N6/c14-13-17-11(9-5-1-3-7-15-9)12(18-19-13)10-6-2-4-8-16-10/h1-8H,
InchiKey:	KRVCKHNYNKZLBH-UHFFFAOYSA-N
Formula:	C13H10N6
SMILES:	Nc1nnc(-c2ccccc2)c(-c2ccccc2)n1
Mol. weight [g/mol]:	250.26
CAS:	116557-76-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	1.578		Crippen Method
mcvol	182.630	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116557767&Units=SI
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

Legend

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

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