

Pyridine, 4-[(s-triazol-3-yl-amino)methyl]-

Inchi:	InChI=1S/C8H9N5/c1-3-9-4-2-7(1)5-10-8-11-6-12-13-8/h1-4,6H,5H2,(H2,10,11,12,13)
InchiKey:	NJSXHDJFNJXUBR-UHFFFAOYSA-N
Formula:	C8H9N5
SMILES:	c1cc(CNc2nc[nH]n2)ccn1
Mol. weight [g/mol]:	175.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.330		Crippen Method
mcvol	130.260	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009187&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

Latest version available from:

<https://www.chemeo.com/cid/66-199-9/Pyridine-4-s-triazol-3-yl-amino-methyl.pdf>

Generated by Cheméo on 2024-04-28 12:15:04.728904579 +0000 UTC m=+16595753.649481896.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.