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/ci990307l
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