

7-Amino-S-triazolo(1,5-a)pyrimidin-5(4H)-one

Other names:	s-Triazolo(1,5-a)pyrimidin-5(4H)-one, 7-amino-(1,2,4)Triazolo(1,5-a)pyrimidin-5(1H)-one, 7-amino-4,5-Dihydro-7-amino-5-oxo-S-triazolo(1,5-a)pyrimidine 7-Amino-S-triazolo[1,5-a]pyrimidine-5(4H)-one
Inchi:	InChI=1S/C5H5N5O/c6-3-1-4(11)9-5-7-2-8-10(3)5/h1-2H,6H2,(H,7,8,9,11)
InchiKey:	JIXZXRNBZVMIQJ-UHFFFAOYSA-N
Formula:	C5H5N5O
SMILES:	<chem>Nc1cc(=O)[nH]c2ncnn12</chem>
Mol. weight [g/mol]:	151.13
CAS:	35186-69-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.24		Crippen Method
logp	-1.482		Crippen Method
mcvol	98.160	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35186697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/47-423-0/7-Amino-S-triazolo-1-5-a-pyrimidin-5-4H-one.pdf>

Generated by Cheméo on 2024-04-26 04:20:11.120846469 +0000 UTC m=+16394460.041423784.

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