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: Nc1cc(=O)[nH]c2ncnn12
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/ci990307l
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

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