

8-Azaguanine

Other names:	7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one, 5-amino-1,4-dihydro- v-Triazolo(4,5-d)pyrimidin-7-ol, 5-amino- Azaguanine Azan Azaguanine, 8 AZG Guanazol Guanazolo NSC-749 Pathocidin Pathocidine SK 1150 Triazologuanine 7H-v-Triazolo(4,5-d)pyrimidin-7-one, 5-amino-1,6-dihydro- 8 AG 5-Amino-1,6-dihydro-7H-v-triazolo(4,5-d)pyrimidin-7-one 5-Amino-1,4-dihydro-7H-1,2,3-triazolo(4,5-d)pyrimidin-7-one 5-Amino-7-hydroxy-1H-v-triazolo(d)pyrimidine 5-Amino-1H-v-triazolo(d)pyrimidin-7-ol B-28 SF-337 NSC 223526 5-amino-1H-triazolo[4,5-d]pyrimidin-7-ol
Inchi:	InChI=1S/C4H4N6O/c5-4-6-2-1(3(11)7-4)8-10-9-2/h(H4,5,6,7,8,9,10,11)
InchiKey:	LPXQRXLUHJKZIE-UHFFFAOYSA-N
Formula:	C4H4N6O
SMILES:	<chem>N=c1nc(O)c2nn[nH]c2[nH]1</chem>
Mol. weight [g/mol]:	152.11
CAS:	134-58-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	-2.098		Crippen Method
mcvol	94.050	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C134587&Units=SI

Legend

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

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