

8-Azaadenine

Other names:	1H-1,2,3-Triazolo[4,5-d]pyrimidin-7-amine Adenine, 8-aza- 1H-v-Triazolo(4,5-d)pyrimidine, 7-amino- 3H-N-Triazolo(4,5-d)pyrimidin-7-amine 6-Amino-8-azapurine 7-Amino-v-triazolo(d)pyrimidine 7-Amino-1-v-triazolo(d)pyrimidine 1H-v-Triazolo(4,5-d)pyrimidin-7-amine 7-Amino-1H-v-triazolo(4,5-d)pyrimidine 8-Azapurine, 6-amino- NSC 32797 7-amino-1H-triazolo[4,5-d]pyrimidine
Inchi:	InChI=1S/C4H4N6/c5-3-2-4(7-1-6-3)9-10-8-2/h1H,(H3,5,6,7,8,9,10)
InchiKey:	HRYKDUPGBWLLHO-UHFFFAOYSA-N
Formula:	C4H4N6
SMILES:	<chem>Nc1ncnc2[nH]nnc12</chem>
Mol. weight [g/mol]:	136.11
CAS:	1123-54-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	-1.152		Crippen Method
mcvol	88.180	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123542&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

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