

3H-v-triazolo[4,5-d]pyrimidine, 5-amino-7-chloro-

Other names:	1H-v-triazolo[4,5-d]pyrimidine, 5-amino-7-chloro-
Inchi:	InChI=1S/C4H3ClN6/c5-2-1-3(10-11-9-1)8-4(6)7-2/h(H3,6,7,8,9,10,11)
InchiKey:	HHVGSWGNKPENEQ-UHFFFAOYSA-N
Formula:	C4H3ClN6
SMILES:	<chem>N=c1nc2[nH]nnc2c(Cl)[nH]1</chem>
Mol. weight [g/mol]:	170.56
CAS:	88780-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	-1.150		Crippen Method
mcvol	100.420	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88780841&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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