

S-triazolo[2,3-c]pyrimidin-2(3h)-one, 8-amino-7-chloro-

Inchi:	InChI=1S/C5H4ClN5O/c6-3-2(7)4-9-5(12)10-11(4)1-8-3/h1H,7H2,(H,10,12)
InchiKey:	KUKJEFXPECNHOR-UHFFFAOYSA-N
Formula:	C5H4ClN5O
SMILES:	<chem>Nc1c(Cl)ncn2nc(O)nc12</chem>
Mol. weight [g/mol]:	185.57
CAS:	15129-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	0.065		Crippen Method
mcvol	110.400	ml/mol	McGowan Method

Sources

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=C15129018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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