

Acetamide, 6(9h)-chloropurine-9-yl-

Inchi:	InChI=1S/C7H6ClN5O/c8-6-5-7(11-2-10-6)13(3-12-5)1-4(9)14/h2-3H,1H2,(H2,9,14)
InchiKey:	IZJHJHPNRBSAAJ-UHFFFAOYSA-N
Formula:	C7H6ClN5O
SMILES:	NC(=O)Cn1cnc2c(Cl)ncnc21
Mol. weight [g/mol]:	211.61
CAS:	98273-93-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	-0.035		Crippen Method
mcvol	134.280	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=C98273939&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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