

6-Chloro-2-ethylpurine

Inchi:	InChI=1S/C7H7ClN4/c1-2-4-11-6(8)5-7(12-4)10-3-9-5/h3H,2H2,1H3,(H,9,10,11,12)
InchiKey:	PMJOANJCPVQPOH-UHFFFAOYSA-N
Formula:	C7H7ClN4
SMILES:	CCc1nc(Cl)c2[nH]cnc2n1
Mol. weight [g/mol]:	182.61
CAS:	1908-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	1.087		Crippen Method
mcvol	122.730	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=C1908232&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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