

Purin-6(1h)-one, 2-chloro-8-chloromethyl-7-methyl-

Inchi:	InChI=1S/C7H6Cl2N4O/c1-13-3(2-8)10-5-4(13)6(14)12-7(9)11-5/h2H2,1H3,(H,11,12,14)
InchiKey:	SMEGPVDLRDXSLQ-UHFFFAOYSA-N
Formula:	C7H6Cl2N4O
SMILES:	Cn1c(CCl)nc2nc(Cl)[nH]c(=O)c21
Mol. weight [g/mol]:	233.06
CAS:	46292-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	0.567		Crippen Method
mcvol	140.840	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C46292824&Units=SI

Legend

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

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