

Formimidic acid, n-6-(chloropurin-2-yl), ethyl ester

Inchi:	InChI=1S/C8H8CIN5O/c1-2-15-4-12-8-13-6(9)5-7(14-8)11-3-10-5/h3-4H,2H2,1H3,(H,10,
InchiKey:	HWIBIPYVLQNYOC-UUILKARUSA-N
Formula:	C8H8CIN5O
SMILES:	CCOC=Nc1nc(Cl)c2[nH]cnc2n1
Mol. weight [g/mol]:	225.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	1.221		Crippen Method
mcvol	148.370	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=B6008266&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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