9H-purine-9-ethanol, 6-chloro-, acetate

Inchi:	InChI=1S/C9H9ClN4O2/c1-6(15)16-3-2-14-5-13-7-8(10)11-4-12-9(7)14/h4-5H,2-3H2,1H3
InchiKey:	WABGFEVHJMMOIL-UHFFFAOYSA-N
Formula:	C9H9ClN4O2
SMILES:	CC(=O)OCCn1cnc2c(Cl)ncnc21
Mol. weight [g/mol]:	240.65
CAS:	6973-54-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	1.043		Crippen Method
mcvol	158.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6973542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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