9H-purine-9-acetic acid, 6-methoxy-

Inchi:	InChI=1S/C8H8N4O3/c1-15-8-6-7(9-3-10-8)12(4-11-6)2-5(13)14/h3-4H,2H2,1H3,(H,13,1
InchiKey:	KXRNTXGADSNVIH-UHFFFAOYSA-N
Formula:	C8H8N4O3
SMILES:	COc1ncnc2c1ncn2CC(=O)O
Mol. weight [g/mol]:	208.17
CAS:	6298-52-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	-0.081		Crippen Method
mcvol	137.890	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6298528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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