Glycine, n-(9h-purin-6-yl)-, ethyl ester

Inchi:	InChI=1S/C9H11N5O2/c1-2-16-6(15)3-10-8-7-9(12-4-11-7)14-5-13-8/h4-5H,2-3H2,1H3,(
InchiKey:	FRWPZDCYVQSDRP-UHFFFAOYSA-N
Formula:	C9H11N5O2
SMILES:	CCOC(=O)CNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	221.22
CAS:	15846-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	-0.154		Crippen Method
mcvol	156.090	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=C15846670&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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