

# 4-Imidazole carboxylic acid, 5[3-(beta-hydroxyethyl)-3-methyl-1-triazeno]-, methyl ester

Inchi: InChI=1S/C8H13N5O3/c1-13(3-4-14)12-11-7-6(8(15)16-2)9-5-10-7/h5,14H,3-4H2,1-2H3,  
InchiKey: NJOLHMNSGBBZOV-VAWYXSNFSA-N

Formula: C8H13N5O3  
SMILES: COC(=O)c1nc[nH]c1N=NN(C)CCO  
Mol. weight [g/mol]: 227.22  
CAS: 36137-85-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	-0.363		Crippen Method
mcvol	163.030	ml/mol	McGowan Method

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C36137856&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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