

4-Imidazolecarboxylic acid, 5-(3-methyltriazen-1-yl)-, methyl ester

Inchi:	InChI=1S/C6H9N5O2/c1-7-11-10-5-4(6(12)13-2)8-3-9-5/h3H,1-2H3,(H,7,10)(H,8,9)
InchiKey:	DENXXPHCWBFNER-UHFFFAOYSA-N
Formula:	C6H9N5O2
SMILES:	CNN=Nc1[nH]cnc1C(=O)OC
Mol. weight [g/mol]:	183.17
CAS:	36137-94-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	-0.068		Crippen Method
mcvol	128.980	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=C36137947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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