

# Methyl 4-(2«lambda»5-1,2-triazadienyl)-1h-imidazole-5-ca

Other names:	Methyl 4-(2«lambda»<5>-1,2-triazadienyl)-1h-imidazole-5-carboxylate
Inchi:	InChI=1S/C5H5N5O2/c1-12-5(11)3-4(9-10-6)8-2-7-3/h2H,1H3,(H,7,8)
InchiKey:	YTQFHDFRUNTVDVDD-UHFFFAOYSA-N
Formula:	C5H5N5O2
SMILES:	COC(=O)c1[nH]cnc1N=[N+]=[N-]
Mol. weight [g/mol]:	167.13
CAS:	50993-51-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.35		Crippen Method
logp	0.656		Crippen Method
mcvol	110.590	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C50993516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50993516&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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