

Imidazole-4-carboxamide, 5-(3'-methyl-1'-triazeno)-

Inchi:	InChI=1S/C5H8N6O/c1-7-11-10-5-3(4(6)12)8-2-9-5/h2H,1H3,(H2,6,12)(H,7,10)(H,8,9)
InchiKey:	MVBPAIHFZZKRGD-UHFFFAOYSA-N
Formula:	C5H8N6O
SMILES:	CNN=Nc1[nH]cnc1C(N)=O
Mol. weight [g/mol]:	168.16
CAS:	3413-72-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.05		Crippen Method
logp	-0.755		Crippen Method
mcvol	119.000	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3413727&Units=SI

Legend

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

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<https://www.chemeo.com/cid/30-227-6/Imidazole-4-carboxamide-5-3-methyl-1-triazeno.pdf>

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