

# 4-Triazolecarboxamide, 5-(3,3-dimethyltriazenyl)-

Inchi:	InChI=1S/C5H9N7O/c1-12(2)11-9-5-3(4(6)13)7-10-8-5/h1-2H3,(H2,6,13)(H,7,8,10)/b11-9
InchiKey:	VHJCJSWMVHEEPX-PKNCBQFBNSA-N
Formula:	C5H9N7O
SMILES:	CN(C)N=Nc1[nH]nnc1C(N)=O
Mol. weight [g/mol]:	183.17
CAS:	46192-24-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	-1.018		Crippen Method
mcvol	128.980	ml/mol	McGowan Method

## Sources

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=C46192249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C46192249&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>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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