

5-[(1E)-3,3-dimethyl-1-triazenyl]-1h-imidazole-4-carbohydrazide

Inchi:	InChI=1S/C6H11N7O/c1-13(2)12-11-5-4(6(14)10-7)8-3-9-5/h3H,7H2,1-2H3,(H,8,9)(H,10)
InchiKey:	JGIJKAROWSLZRI-VAWYXSNFSA-N
Formula:	C6H11N7O
SMILES:	CN(C)N=Nc1[nH]cnc1C(=O)NN
Mol. weight [g/mol]:	197.20
CAS:	116401-55-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	-0.908		Crippen Method
mcvol	143.070	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116401559&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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