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-PKNBQFBNSA-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: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C46192249&Units=SI

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

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