Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazeno)-

Other names:	dacarbazine
Inchi:	InChI=1S/C6H10N6O/c1-12(2)11-10-6-4(5(7)13)8-3-9-6/h3H,1-2H3,(H2,7,13)(H,8,9)/b11
InchiKey:	FDKXTQMXEQVLRF-ZHACJKMWSA-N
Formula:	C6H10N6O
SMILES:	CN(C)N=Nc1[nH]cnc1C(N)=O
Mol. weight [g/mol]:	182.18
CAS:	4342-03-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.85		Crippen Method
logp	-0.413		Crippen Method
mcvol	133.090	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=C4342034&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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