

Imidazole-4-carboxamide, 5-(3-methyl-3-phenyltriazeno)-

Inchi:	InChI=1S/C11H12N6O/c1-17(8-5-3-2-4-6-8)16-15-11-9(10(12)18)13-7-14-11/h2-7H,1H3,
InchiKey:	SNBKXSKCAJBZJK-FOCLMDBBSA-N
Formula:	C11H12N6O
SMILES:	CN(N=Nc1[nH]cnc1C(N)=O)c1ccccc1
Mol. weight [g/mol]:	244.25
CAS:	20460-79-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.162		Crippen Method
mcvol	179.780	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=C20460791&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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