

4-Imidazole carboxamide,5-(3-methyl-3-pentyl-1-triazeno)-

Inchi:	InChI=1S/C10H18N6O/c1-3-4-5-6-16(2)15-14-10-8(9(11)17)12-7-13-10/h7H,3-6H2,1-2H1
InchiKey:	GYKARXVGMYBIQL-CCEZHUSRSA-N
Formula:	C10H18N6O
SMILES:	CCCCCN(C)N=Nc1[nH]cnc1C(N)=O
Mol. weight [g/mol]:	238.29
CAS:	18910-61-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.147		Crippen Method
mcvol	189.450	ml/mol	McGowan Method

Sources

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=C18910617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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