

4-Imidazolecarboxylic acid, 5-(dimethyl-1-triazeno)-, butyl ester

Inchi:	InChI=1S/C10H17N5O2/c1-4-5-6-17-10(16)8-9(12-7-11-8)13-14-15(2)3/h7H,4-6H2,1-3H1
InchiKey:	ZPCAGCXFSKUPRF-BUHFOSPRSA-N
Formula:	C10H17N5O2
SMILES:	CCCCOC(=O)c1nc[nH]c1N=NN(C)C
Mol. weight [g/mol]:	239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	1.445		Crippen Method
mcvol	185.340	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=B6008211&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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