

4-Imidazolecarboxylic acid, 5-(dibutyl-1-triazeno)-, methyl ester

Inchi:	InChI=1S/C13H23N5O2/c1-4-6-8-18(9-7-5-2)17-16-12-11(13(19)20-3)14-10-15-12/h10H
InchiKey:	NJSKALMPRJQVKZ-WUKNDPDISA-N
Formula:	C13H23N5O2
SMILES:	CCCCN(CCCC)N=Nc1[nH]cnc1C(=O)OC
Mol. weight [g/mol]:	281.35
CAS:	36295-91-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.615		Crippen Method
mcvol	227.610	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=C36295917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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