

Imidazole-4-carboxylic acid, 5-(3-methyl-3-octyltriazeno)-, ethyl ester

Inchi:	InChI=1S/C15H27N5O2/c1-4-6-7-8-9-10-11-20(3)19-18-14-13(16-12-17-14)15(21)22-5-2
InchiKey:	UZCDEAXDOMDAEL-VHEBQXMUSA-N
Formula:	C15H27N5O2
SMILES:	CCCCCCCCN(C)N=Nc1[nH]cnc1C(=O)OCC
Mol. weight [g/mol]:	309.41
CAS:	36137-96-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.396		Crippen Method
mcvol	255.790	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=C36137969&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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