

Imidazole-4-carboxylic acid, 5-(3-cyclohexyl-3-methyl-1-triazeno)-, 2-(diethylamino)ethyl ester

InChI: 1SC17H30N6O2/c1-4-23(5-2)11-12-25-17(24)15-16(19-13-18-15)20-21-22(3)14-9
InChIKey: UYSTZEPJRJFPGF-QZQOTICOSA-N

Formula: C17H30N6O2
SMILES: CCN(CC)CCOC(=O)c1nc[nH]c1N=NN(C)C1CCCCC1
Mol. weight [g/mol]: 350.46
CAS: 36142-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.690		Crippen Method
mcvol	283.090	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=C36142606&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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