

5-(3'-Methyl-3'-cyclohexyl-1'-triazeno)imidazole-4-carboxylic acid, ethyl ester

InChI: CCOC(=O)c1nc[nH]c1N=NN(C)C1CCCCC1
InChIKey: SSZJUMIEXBBWBQ-WUKNDPDISA-N

Formula: C₁₃H₂₁N₅O₂
SMILES: CCOC(=O)c1nc[nH]c1N=NN(C)C1CCCCC1
Mol. weight [g/mol]: 279.34
CAS: 36137-87-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	2.368		Crippen Method
mcvol	216.750	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=C36137878&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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