Propanoic acid, 2-[(4-aminocarbonylimidazol-5-yl)-1-triazen-1,3-di ethyl ester

InChI: InChI=1S/C9H14N6O3/c1-3-18-9(17)5(2)13-15-14-8-6(7(10)16)11-4-12-8/h4-5H,3H2,1-2

InChIKey: RPUCQYZSMSACIV-UHFFFAOYSA-N

Formula: C9H14N6O3

SMILES: CCOC(=O)C(C)NN=Nc1[nH]cnc1C(N)=O

Mol. weight [g/mol]: 254.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	-0.433		Crippen Method
mcvol	182.800	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010468&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/13-357-1/Propanoic-acid-2-4-aminocarbonylimidazol-5-yl-1-triazen-1-3-diyl-ethyl-ester.p
Generated by Cheméo on 2024-04-19 18:07:13.712087957 +0000 UTC m=+15839282.632665269.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.