

Acetic acid, [3-(4-carbamoylimidazol-5-yl)-2-triazeno]-, ethyl ester

InChI: InChI=1S/C8H12N6O3/c1-2-17-5(15)3-12-14-13-8-6(7(9)16)10-4-11-8/h4H,2-3H2,1H3,(H
InChIKey: TXNGTDMYUCCJRY-UHFFFAOYSA-N
Formula: C8H12N6O3
SMILES: CCOC(=O)CNN=Nc1[nH]cnc1C(N)=O
Mol. weight [g/mol]: 240.22
CAS: 3413-78-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	-0.822		Crippen Method
mvol	168.710	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=C3413783&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
mvol: McGowan's characteristic volume

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