Glycine, n-(1-aziridinylcarbonyl)-, ethyl ester

Inchi: InChI=1S/C7H12N2O3/c1-2-12-6(10)5-8-7(11)9-3-4-9/h2-5H2,1H3,(H,8,11)
InchiKey: BDNXTQQHSJPSOH-UHFFFAOYSA-N
Formula: C7H12N2O3
SMILES: CCOC(=O)CNC(=O)N1CC1
Mol. weight [g/mol]: 172.18
CAS: 98337-03-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.02		Crippen Method
logp	-0.425		Crippen Method
mcvol	127.600	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=C98337032&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