

Glycine, N-(3-pyridinylcarbonyl)-, methyl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C9H10N2O3/c1-14-8(12)6-11-9(13)7-3-2-4-10-5-7/h2-5H,6H2,1H3,(H,11,13) |
| InchiKey: | YZFCSHLOLUYQKO-UHFFFAOYSA-N |
| Formula: | C9H10N2O3 |
| SMILES: | COC(=O)CNC(=O)c1cccnc1 |
| Mol. weight [g/mol]: | 194.19 |
| CAS: | 57397-47-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.28 | | Crippen Method |
| logp | -0.016 | | Crippen Method |
| mcvol | 142.880 | ml/mol | McGowan Method |
| rinpole | 1634.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C57397474&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| rinpole: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/19-630-1/Glycine-N-3-pyridinylcarbonyl-methyl-ester.pdf>

Generated by Cheméo on 2024-04-25 15:02:00.455821816 +0000 UTC m=+16346569.376399127.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.