

Glycin, N-(5-methoxycarbonylfuroyl), methyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C9H11NO5/c1-13-7(11)5-10-9(12)6-3-4-8(14-2)15-6/h3-4H,5H2,1-2H3,(H,10,1 |
| InchiKey: | PTDOFMIGXLBNOE-UHFFFAOYSA-N |
| Formula: | C9H11NO5 |
| SMILES: | COC(=O)CNC(=O)c1ccc(OC)o1 |
| Mol. weight [g/mol]: | 213.19 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.37 | | Crippen Method |
| logp | 0.191 | | Crippen Method |
| mcvol | 148.940 | ml/mol | McGowan Method |
| rinpol | 1845.00 | | NIST Webbook |
| rinpol | 1845.00 | | NIST Webbook |

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=R106619&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 |
| rinpol: | Non-polar retention indices |

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<https://www.chemeo.com/cid/63-666-3/Glycin-N-5-methoxycarbonylfuroyl-methyl-ester.pdf>

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