

Pipecolylpipecolic acid, N-butoxycarbonyl-, isobutyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C21H36N2O5/c1-4-5-14-27-21(26)23-13-9-6-10-17(23)19(24)22-12-8-7-11-18 |
| InchiKey: | AAXCFZXGXFSJDU-UHFFFAOYSA-N |
| Formula: | C21H36N2O5 |
| SMILES: | CCCCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCC(C)C |
| Mol. weight [g/mol]: | 396.52 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.00 | | Crippen Method |
| logp | 3.358 | | Crippen Method |
| mcvol | 321.440 | ml/mol | McGowan Method |
| rinpol | 2629.00 | | NIST Webbook |
| rinpol | 2629.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393064&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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 |
| rinpol: | Non-polar retention indices |

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