

Pipecolylpipecolic acid, N-ethoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C17H28N2O5/c1-3-23-16(21)14-10-6-7-11-18(14)15(20)13-9-5-8-12-19(13)17
InchiKey: YAOOBWQFMDIAOS-UHFFFAOYSA-N
Formula: C17H28N2O5
SMILES: CCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 340.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.57 | | Crippen Method |
| logp | 1.942 | | Crippen Method |
| mcvol | 265.080 | ml/mol | McGowan Method |
| rinpole | 2390.00 | | NIST Webbook |
| rinpole | 2390.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393080&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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