

Isonipecotic acid, N-isobutoxycarbonyl-, ethyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C13H23NO4/c1-4-17-12(15)11-5-7-14(8-6-11)13(16)18-9-10(2)3/h10-11H,4-9H |
| InchiKey: | WIPKODJYUYCDAN-UHFFFAOYSA-N |
| Formula: | C13H23NO4 |
| SMILES: | CCOC(=O)C1CCN(C(=O)OCC(C)C)CC1 |
| Mol. weight [g/mol]: | 257.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.95 | | Crippen Method |
| logp | 2.054 | | Crippen Method |
| mcvol | 208.030 | ml/mol | McGowan Method |
| rinsol | 1808.00 | | NIST Webbook |
| rinsol | 1808.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U322060&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinsol: | Non-polar retention indices |

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