

Isonipecotic acid, N-(3-methoxybenzoyl)-, isobutyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C18H25NO4/c1-13(2)12-23-18(21)14-7-9-19(10-8-14)17(20)15-5-4-6-16(11-15 |
| InchiKey: | DJMNMFDEFIWKBA-UHFFFAOYSA-N |
| Formula: | C18H25NO4 |
| SMILES: | COc1cccc(C(=O)N2CCC(C(=O)OCC(C)C)CC2)c1 |
| Mol. weight [g/mol]: | 319.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.36 | | Crippen Method |
| logp | 2.747 | | Crippen Method |
| mcvol | 254.720 | ml/mol | McGowan Method |
| rinpola | 2645.00 | | 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=U361174&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

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

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