

N-(5-Bromopentyl)phthalimide

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|-----------------------------|--|
| Inchi: | InChI=1S/C13H14BrNO2/c14-8-4-1-5-9-15-12(16)10-6-2-3-7-11(10)13(15)17/h2-3,6-7H, |
| InchiKey: | QKVHAKICMNABGB-UHFFFAOYSA-N |
| Formula: | C13H14BrNO2 |
| SMILES: | O=C1c2ccccc2C(=O)N1CCCCCBr |
| Mol. weight [g/mol]: | 296.16 |
| CAS: | 954-81-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.93 | | Crippen Method |
| logp | 2.848 | | Crippen Method |
| mcvol | 190.030 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C954814&Units=SI |

Legend

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

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