

4-Butylbenzoic acid, morpholide

Inchi: InChI=1S/C15H21NO2/c1-2-3-4-13-5-7-14(8-6-13)15(17)16-9-11-18-12-10-16/h5-8H,2-4
InchiKey: MSGZJSXSKGWKSZ-UHFFFAOYSA-N
Formula: C15H21NO2
SMILES: CCCCc1ccc(C(=O)N2CCOCC2)cc1
Mol. weight [g/mol]: 247.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.07 | | Crippen Method |
| logp | 2.502 | | Crippen Method |
| mcvol | 205.010 | ml/mol | McGowan Method |
| rinpole | 2083.00 | | NIST Webbook |
| rinpole | 2083.00 | | 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=U306999&Units=SI>

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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