

3-(Beta-morpholinoethyl)-3-phenyl-2-benzofurano

Inchi: InChI=1S/C20H21NO3/c22-19-20(16-6-2-1-3-7-16,10-11-21-12-14-23-15-13-21)17-8-4-5
InchiKey: NGAHPZMFYXWQOI-UHFFFAOYSA-N
Formula: C20H21NO3
SMILES: O=C1Oc2ccccc2C1(CCN1CCOCC1)c1ccccc1
Mol. weight [g/mol]: 323.39
CAS: 95696-17-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.10 | | Crippen Method |
| logp | 2.614 | | Crippen Method |
| mcvol | 246.710 | 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=C95696176&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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