

Benzoyl-furoyl

Inchi: InChI=1S/C12H8O3/c13-11(9-5-2-1-3-6-9)12(14)10-7-4-8-15-10/h1-8H
InchiKey: RRHBYDSLXIHTGW-UHFFFAOYSA-N
Formula: C12H8O3
SMILES: O=C(C(=O)c1ccco1)c1ccccc1
Mol. weight [g/mol]: 200.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	2.345		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
rinpol	1660.00		NIST Webbook
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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=R121143&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/94-019-7/Benzoyl-furoyl.pdf>

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