

Furan, 2-[(2-furyl)-(phenylamino)methylcarbonyl]

Inchi: InChI=1S/C16H13NO3/c18-16(14-9-5-11-20-14)15(13-8-4-10-19-13)17-12-6-2-1-3-7-12/
InchiKey: ZOIWPXRLGKGGKK-UHFFFAOYSA-N
Formula: C16H13NO3
SMILES: O=C(c1ccco1)C(Nc1ccccc1)c1ccco1
Mol. weight [g/mol]: 267.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.91		Crippen Method
logp	3.909		Crippen Method
mcvol	196.910	ml/mol	McGowan Method
rinpole	2104.00		NIST Webbook
rinpole	2104.00		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=R121212&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

Latest version available from:

<https://www.cheméo.com/cid/113-728-8/Furan-2-2-furyl-phenylamino-methylcarbonyl.pdf>

Generated by Cheméo on 2024-05-01 04:38:51.033250655 +0000 UTC m=+16827579.953827968.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.