

Furan, 2-[(2-furyl)-(4-methylphenylamino)methylcarbonyl

Inchi: InChI=1S/C17H15NO3/c1-12-6-8-13(9-7-12)18-16(14-4-2-10-20-14)17(19)15-5-3-11-21-
InchiKey: GGWLLACYWSQUKT-UHFFFAOYSA-N
Formula: C17H15NO3
SMILES: Cc1ccc(NC(C(=O)c2ccco2)c2ccco2)cc1
Mol. weight [g/mol]: 281.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.39		Crippen Method
logp	4.217		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R121207&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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