

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

Inchi: InChI=1S/C16H12ClNO3/c17-11-5-7-12(8-6-11)18-15(13-3-1-9-20-13)16(19)14-4-2-10-2
InchiKey: LGYDLBCDQLSDFR-UHFFFAOYSA-N
Formula: C16H12ClNO3
SMILES: O=C(c1ccco1)C(Nc1ccc(Cl)cc1)c1ccco1
Mol. weight [g/mol]: 301.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.60		Crippen Method
logp	4.562		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
rinpole	2330.00		NIST Webbook

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=R121198&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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