

Acetophenone, 2-(2-furyl)-(4-methylphenylamino)

Inchi: InChI=1S/C19H17NO2/c1-14-9-11-16(12-10-14)20-18(17-8-5-13-22-17)19(21)15-6-3-2-4
InchiKey: ARCXFPWIBBPBTC-UHFFFAOYSA-N
Formula: C19H17NO2
SMILES: Cc1ccc(NC(C(=O)c2ccccc2)c2ccco2)cc1
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.65		Crippen Method
logp	4.624		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
rinpola	2352.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R121103&Units=SI>
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>

Legend

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

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