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
rinpol	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/ci990307l

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

rinpol: Non-polar retention indices