

# 1-(p-(Dimethylamino)phenyl)-2-(2-furyl)ethanedione

<b>Other names:</b>	1-[4-(Dimethylamino)phenyl]-2-(2-furyl)-1,2-ethanedione Furoyl, 4-dimethylaminobenzoyl
<b>Inchi:</b>	InChI=1S/C14H13NO3/c1-15(2)11-7-5-10(6-8-11)13(16)14(17)12-4-3-9-18-12/h3-9H,1-2
<b>InchiKey:</b>	PHALNKSJQMXERZ-UHFFFAOYSA-N
<b>Formula:</b>	C14H13NO3
<b>SMILES:</b>	CN(C)c1ccc(C(=O)C(=O)c2ccco2)cc1
<b>Mol. weight [g/mol]:</b>	243.26
<b>CAS:</b>	28123-26-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	2.411		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C28123264&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28123264&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/45-192-9/1-p-Dimethylamino-phenyl-2-2-furyl-ethanedione.pdf>

Generated by Cheméo on 2024-04-25 16:12:23.165556541 +0000 UTC m=+16350792.086133857.

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