1-(p-(Dimethylamino)phenyl)-2-(2-furyl)ethanedio

Other names:	1-[4-(Dimethylamino)phenyl]-2-(2-furyl)-1,2-ethanedione
	Furoyl, 4-dimethylaminobenzoyl
Inchi:	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
InchiKey:	PHALNKSJQMXERZ-UHFFFAOYSA-N
Formula:	C14H13NO3
SMILES:	CN(C)c1ccc(C(=O)C(=O)c2ccco2)cc1
Mol. weight [g/mol]:	243.26
CAS:	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28123264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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