

1,3-dimethyl-5,5-diphenyl-1,3-diazinane-2,4,6-trione

Inchi:	InChI=1S/C18H16N2O3/c1-19-15(21)18(13-9-5-3-6-10-13,14-11-7-4-8-12-14)16(22)20(2)
InchiKey:	FIRNIXWQYFVBKZ-UHFFFAOYSA-N
Formula:	C18H16N2O3
SMILES:	CN1C(=O)N(C)C(=O)C(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]:	308.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.023		Crippen Method
mcvol	230.770	ml/mol	McGowan Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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