5-Methyl-2,4-diphenyl-1,2,4-triazol-3-one

Inchi: InChI=1S/C15H13N3O/c1-12-16-18(14-10-6-3-7-11-14)15(19)17(12)13-8-4-2-5-9-13/h2-1
InchiKey: JCJVMCXFZOETTE-UHFFFAOYSA-N
Formula: C15H13N3O
SMILES: Cc1nn(-c2ccccc2)c(=O)n1-c1ccccc1
Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	2.332		Crippen Method
mcvol	191.040	ml/mol	McGowan Method
rinpol	2031.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R577898&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