

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-
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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/41-202-1/5-Methyl-2-4-diphenyl-1-2-4-triazol-3-one.pdf>

Generated by Cheméo on 2024-04-28 11:02:17.492558533 +0000 UTC m=+16591386.413135850.

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