

3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine

Other names:	5,6-Diphenyl-3-(2-pyridyl)-1,2,4-triazine 1,2,4-Triazine, 5,6-diphenyl-3-(2-pyridinyl)- as-Triazine, 5,6-diphenyl-3-(2-pyridyl)-
Inchi:	InChI=1S/C20H14N4/c1-3-9-15(10-4-1)18-19(16-11-5-2-6-12-16)23-24-20(22-18)17-13-7
InchiKey:	OTMYLOBWDNFTLO-UHFFFAOYSA-N
Formula:	C20H14N4
SMILES:	c1ccc(-c2nnc(-c3ccccc3)nc2-c2ccccc2)cc1
Mol. weight [g/mol]:	310.35
CAS:	1046-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	4.268		Crippen Method
mcvol	237.540	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1046566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/33-013-0/3-2-Pyridyl-5-6-diphenyl-1-2-4-triazine.pdf>

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