

# 3-Anilino-1,4-diphenyl-5-phenylimino-1,2,4-triazol

<b>Inchi:</b>	InChI=1S/C26H21N5/c1-5-13-21(14-6-1)27-25-29-31(24-19-11-4-12-20-24)26(28-22-15-
<b>InchiKey:</b>	STYFIGFBShzrbk-BYCLXTJYSA-N
<b>Formula:</b>	C26H21N5
<b>SMILES:</b>	c1ccc(N=c2n(-c3ccccc3)nc(Nc3ccccc3)n2-c2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	403.48
<b>CAS:</b>	5416-43-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	5.639		Crippen Method
mcvol	312.600	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5416433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5416433&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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