

4H-1,2,4-Triazole, 3,4,5-triphenyl-

Other names:	3,4,5-Triphenyl-1,2,4-triazole
Inchi:	InChI=1S/C20H15N3/c1-4-10-16(11-5-1)19-21-22-20(17-12-6-2-7-13-17)23(19)18-14-8-3
InchiKey:	LLTSIOOHJBUDCP-UHFFFAOYSA-N
Formula:	C20H15N3
SMILES:	<chem>c1ccc(-c2nnc(-c3ccccc3)n2-c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	297.35
CAS:	4073-72-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	4.601		Crippen Method
mcvol	231.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4073727&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

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