

1,2,4,5-Tetrazine, 3,6-diphenyl-

Other names:	Diphenyl-s-tetrazine 3,6-Diphenyltetrazine 3,6-Diphenyl-s-tetrazine 3,6-Diphenyl-sym-tetrazine 3,6-Diphenyl-1,2,4,5-tetrazine s-Tetrazine, 3,6-diphenyl-
Inchi:	InChI=1S/C14H10N4/c1-3-7-11(8-4-1)13-15-17-14(18-16-13)12-9-5-2-6-10-12/h1-10H
InchiKey:	XAUWSIIGUUMHQQ-UHFFFAOYSA-N
Formula:	C14H10N4
SMILES:	<chem>c1ccc(-c2nnc(-c3ccccc3)nn2)cc1</chem>
Mol. weight [g/mol]:	234.26
CAS:	6830-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	2.601		Crippen Method
mcvol	176.760	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6830780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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