

1,3,5-Triazine, 2,4,6-triphenyl-

Other names:	s-Triazine, 2,4,6-triphenyl- Cyaphenine Kyaphenine Triphenyl-s-triazine 2,4,6-Triphenyl-s-triazine 2,4,6-Triphenyl-1,3,5-triazine 2,4,6-Triphenyltriazine S-Triphenyltriazine NSC 46521
Inchi:	InChI=1S/C21H15N3/c1-4-10-16(11-5-1)19-22-20(17-12-6-2-7-13-17)24-21(23-19)18-14
InchiKey:	HBQUOLGAXBYZGR-UHFFFAOYSA-N
Formula:	C21H15N3
SMILES:	<chem>c1ccc(-c2nc(-c3ccccc3)nc(-c3ccccc3)n2)cc1</chem>
Mol. weight [g/mol]:	309.36
CAS:	493-77-6

Physical Properties

Property code	Value	Unit	Source
chs	-10689.70 ± 6.30	kJ/mol	NIST Webbook
hfs	282.70 ± 6.30	kJ/mol	NIST Webbook
log10ws	-8.58		Crippen Method
logp	4.873		Crippen Method
mcvol	241.650	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=C493776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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