

# 1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexachloro-2,2,4,4,6,6-hexahydro-

<b>Other names:</b>	1,3,5,2,4,6-Triazatriphosphorine, hexachloro- 2,2,4,4,6,6-Hexachlorocyclotriphosphazatriene 2,2,4,4,6,6-hexachloro-1,3,5-triaza-2,4,6-triphosphorine 2«lambda»5,4«lambda»5,6«lambda»5-1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexachloro- Cyclophosphazene dichloride trimer Cyclophosphonitrilic chloride trimer Hexachloro-1,3,5,2,4,6-triazatriphosphorine Hexachlorocyclophosphazatriene Hexachlorocyclotriphosphazatriene Hexachlorotriphosphazene Hexachlorotriphosphonitrile NSC 209799 NSC 2667 Phosphonitrile chloride, cyclic trimer Phosphonitrilic chloride cyclic trimer Phosphonitrilic chloride trimer Phosphononitrilic chloride trimer Triphosphonitrile chloride Triphosphonitrilic chloride hexachlorocyclotriphosphazene
<b>Inchi:</b>	InChI=1S/Cl6N3P3/c1-10(2)7-11(3,4)9-12(5,6)8-10
<b>InchiKey:</b>	UBIJTWDKTYCPMQ-UHFFFAOYSA-N
<b>Formula:</b>	Cl6N3P3
<b>SMILES:</b>	CIP1(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=N1
<b>Mol. weight [g/mol]:</b>	347.66
<b>CAS:</b>	940-71-6

## Physical Properties

Property code	Value	Unit	Source
hfus	19.61	kJ/mol	Solubilities of Phenylphosphinic Acid, Methylphenylphosphinic Acid, Hexachlorocyclotriphosphazene, and Hexaphenoxycyclotriphosphazene in Selected Solvents
ie	10.05 ± 0.03	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook

ie	10.26 ± 0.05	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
log10ws	3.84		Crippen Method
logp	7.271		Crippen Method
mcvol	164.760	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.50	kJ/mol	388.60	NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C940716&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Solubilities of Phenylphosphinic Acid, Methylphenylphosphinic Acid, Methylphenylphosphonic Acid, and Hexaphenoxycyclotriphosphazene in Selected Solvents:** <https://www.doi.org/10.1021/je1009812>

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>ie:</b>	Ionization energy
<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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