

1,3,5,7,2,4,6,8-Tetrazatetraphosphocine, 2,2,4,4,6,6,8,8-octachloro-2,2,4,4,6,6,8,8-octahydro

Other names:	Nitrogen chloride phosphide ((NPCl ₂) ₄) Octachlorocyclophosphazetetraene Octachlorocyclotetraphosphazetetraene Octachlorocyclotetraphosphazene Octachlorotetraphosponitrile Phosponitrile chloride, cyclic tetramer Phosponitrile chloride, tetramer Phosponitrilic chloride cyclic tetramer Tetraphosponitrile chloride 1,1,3,3,5,5,7,7-Octachlorocyclotetraphosphaza-1,3,5,7-tetraene Tetraphosponitrilic chloride Cyclo-tetrakis(dichlorophosponitrile) 2,2,4,4,6,6,8,8-Octachloro-2,2,4,4,6,6,8,8-octahydro-1,3,5,7,2,4,6,8-tetraazatetraphosphocine 2,2,4,4,6,6,8,8-octachloro-1,3,5,7,2,4,6,8-tetraazatetraphosphocine N ₄ C ₄ P ₄ Cl ₈
Inchi:	InChI=1S/Cl ₈ N ₄ P ₄ /c1-13(2)9-14(3,4)11-16(7,8)12-15(5,6)10-13
InchiKey:	PEJQKHLWXHKKGS-UHFFFAOYSA-N
Formula:	Cl ₈ N ₄ P ₄
SMILES:	CIP1(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=NP(Cl)(Cl)=N1
Mol. weight [g/mol]:	463.55
CAS:	2950-45-0

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.05	eV	NIST Webbook
log10ws	5.03		Crippen Method
logp	9.695		Crippen Method
mcvol	219.680	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.20	kJ/mol	400.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2950450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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