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Phosphorus oxychloride, 99%

ACROS
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MSDS Specifications Applications Categories 3D model Infrared Molfile



General

Product Name Phosphorus oxychloride
Phosphoryl chloride

CAS RN 10025-87-3

ACD Code MFCD00011443

Structure

Molecular Formula Cl₃ O P

Molecular weight 153.33

Pack size	Catalog	Qty / UM	Price (EUR)
	191290010	1 KG	65.10 Order Check stock
	191292500	250 GR	28.90 Order Check stock

Physical

Density (g/cm³) 1.645
 Refractive index 1.46 - 1.462
 Boiling Point (°C) 107
 Melting Point (°C) 1.2

Safety

GHS Pictogram

GHS Signal Word Danger

GHS H statement
 H330: Fatal if inhaled
 H372: Causes damage to organs through prolonged or repeated exposure
 H314: Causes severe skin burns and eye damage
 H302: Harmful if swallowed
 EUH029: Contact with water liberates toxic gas
 EUH014: Reacts violently with water

GHS P statement
 P301 + P330 + P331: IF SWALLOWED: rinse mouth. Do NOT induce vomiting
 P280: Wear eye protection/face protection
 P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 P304 + P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 P260: Do not breathe dust/fume/gas/mist/vapors/spray

Hazard
 T+: Very toxic
 C: Corrosive

Risk
 14: Reacts violently with water.
 22: Harmful if swallowed.
 26: Very toxic by inhalation.
 29: Contact with water liberates toxic gas.
 35: Causes severe burns.
 48/23: Toxic : danger of serious damage to health by prolonged exposure through inhalation.

Safety
 7/8: Keep container tightly closed and dry.
 26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
 36/37/39: Wear suitable protective clothing, gloves and eye/face protection.
 45: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Categories

Preparation, Purification and Analysis > Routine Reagents
 Functional Reagents > Oxidation > Others
 Functional Reagents > C-X Bond Formation (Halogen) > Chlorination

Applications						
	Function	Transformation		Type	Caveat	Reference
	Reagent	Aromatic electrophilic substitution		Formylation	Vilsmeier reagents, typically POCl3/ DMF.	T 1992, 48, 3659; FF 1967, 1, 876; COS 1991, 2, 777
	Reagent	Aromatic electrophilic substitution		Ring formation via Bischler-Napieralski synthesis	Substituted amides to dihydroisoquinolines.	TL 1985, 26, 5975
	Reagent	Dehydration		Alcohol to alkene	POCl3/ pyridine.	JACS 1986, 108, 3443
	Reagent	Dehydration		N-Formamide to isocyanide	Typically an amine base or Potassium t-Butoxide is also required.	Sandler, S. R.; Karo, W. In Organic Functional Group Preparations 2nd ed.; Academic: San Diego, 1989; Vol. 3, pp 207-238
	Reagent	Dehydration		Primary amide to nitrile		Bieron; Dinan; in Zabicky The chemistry of Amides; Wiley: New York, 1970; pp 274-283
	Reagent	Halogenation		Alcohol to alkyl halide	POCl3/ DMF, POCl3 alone will phosphorylate.	S 1980, 746
	Reagent	Halogenation		Heterocyclic ketones	e.g. a pyrimidone to a chloropyrimidine.	JHC 1985, 22, 601
	Reagent	Halogenation		Phenols to haloarenes		
	Reagent	phosphorylation agent		amines, thiols and primary alcohols	2° and 3° alcohols convert to chloro.	COS 1991, 6, 601
Reagent	Rearrangements		Beckmann	Ketoximes to amides.	S 1982, 68	
Other						
Infrared	Show					
Parameter	EINECS	233-046-7				
	Solubility	Solubility in water: Decomposes				Solubility in other solvents: Soluble in CCl4, chloroform and benzene
	Origin	synthetic				
	References:	Electrical conductivities of poly(alkyl vinyl ketones)reacted with dopant solutions. Ma, Jun Hui; Tauber, J. David;Ramelow, Ulku S.Turk. J. Chem., 21(4), 313-326, 1997.Dopant diffusion in silicon and polysilicon using phosphorusoxychloride (POCl3). Roy, Sudipto R.; Haji-Sheikh, A.HTD (Am. Soc. Mech. Eng.), 323(ASME Proceedings of the31st National Heat Transfer Conference, 1996, Vol. 1), 247-253, 1996.Preparation of monoalkyl phosphate of secondary alcohol.Hiyama, Keiichiro et al.;Kagaku to Kogyo (Osaka), 72(3), 89-94, 1998.				
	Literature					
	Reference:	01,876; 02,330; 03,228; 04,390; 05,535; 07,292; 09,374; 11,429; 13,249; 15,267; 17,288				
	Fieser					
	Reference:	15,7461				
	Merck					
3D model	Show					