



tert-BUTYLDICHLOROPHOSPHINE (TBDCP)

CAS No. 25979-07-1

QS-PDS-027 Revision: 00

Product Name *tert*-Butyldichlorophosphine, *t*-Butyldichlorophosphine, TBDCP

Formula C₄H₉PCl₂

Appearance White Solid. In heptane, it is a colorless to light yellow or green solution.

Application *tert*-Butyldichlorophosphine (TBDCP) is used primarily in the preparation of mono- and bidentate phosphine ligands in metal complexes for catalytic chiral asymmetric hydrogenations and other asymmetric reactions as well as transition metal coupling reactions. This reagent is also used in the preparation of other phosphines in catalytic polymerization reactions. For reviews see: 1) *Palladium Reagents and Catalysts*, John Wiley & Sons: Chichester, **1995** p.345-356. 2) *Advanced Synthesis & Catalysis*, Wiley-VCH Verlag GmbH **2001** p.118-136. 3) *Tetrahedron: Asymmetry* **2004**, 15 (17), 2621-2631 and references cited therein.

Product Specification

tert-Butyldichlorophosphine
Purity by ³¹P NMR, %

Guaranteed*

40 – 100 wt.% in hydrocarbon sol.
95 min

* This product can be made to agreed upon customer specifications

Physical Properties

Molecular weight	158.99
Melting point	44 – 49°C (neat solid)
Boiling point	145°C (98°C for heptane)
Percent volatile	<1% excluding solvent
Pyrophoricity	Non-pyrophoric

Solubility *tert*-Butyldichlorophosphine is infinitely soluble in hydrocarbon and ethereal solvents.

Thermal Stability *tert*-Butyldichlorophosphine is thermally stable, experimentally determined to 220°C.





tert-BUTYLDICHLOROPHOSPHINE (TBDP)

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Toxicity/Safety Data

Corrosive solution. Reacts violently with water. Handle under nitrogen or inert gas. Reacts slowly with moisture to form hydrogen chloride and phosphorus oxides.

Corrosive to eyes (may cause blindness), skin, mucous membranes and upper respiratory tract. Harmful if swallowed, inhaled, or adsorbed through skin. Lachrymator. Stench.

COMPLETE INFORMATION ON TOXICITY AND SAFETY IS CONTAINED IN THE OPTIMA MATERIAL SAFETY DATA SHEET (MSDS) AVAILABLE FOR THIS PRODUCT.

Handling/Storage/Disposal

Do not get in eyes, on skin or clothing. Wash thoroughly after handling. Use in a closed system under argon or nitrogen.

Keep away from heat, sparks and flame. Keep container tightly closed. Use and store under argon or nitrogen.

Shipping Containers

Cylinders	#5 – 420 L
Glass bottles	125 mL, 500 mL and 1 L

Shipping Limitations

Shipments of *tert*-Butyldichlorophosphine are described as Corrosive Solid, Acidic, Organic, N.O.S. (*TERT-BUTYLDICHLOROPHOSPHINE*) 8, UN3261 PG II." Shipments require a "Corrosive" label.

Post, Parcel	Forbidden
Sea	Class 8 (IMDG)
Road, Rail	Class 8 (DOT, RID/ADR)
Air	Class 8 (IATA) Cargo Aircraft
	2.5 kg maximum per inner glass container.
	5.0 kg maximum per metal container.
	50 kg maximum per outer package

For shipments within Europe, labeling for supply requirements are:

C	Corrosive
R&S Phrases	See Material Safety Data Sheet

Responsible Care® initiative dictates that all shipments must be transported in a DOT-approved vehicle in a responsible manner (i.e., no flat bed trucks).

Additional Resources

Refer to the Organometallics and Reactive Specialty Organics Safe Handling Guide.