



DI-*t*-BUTYLNEOPENTYLPHOSPHONIUM HBF₄ SALT

CAS No. 886059-84-3

QS-PDS-028 Revision: 00

Product Name Di-*tert*-butylneopentylphosphonium tetrafluoroborate, DTBNpP.HBF₄

Formula C₁₃H₃₀BF₄P

Appearance White solid

Application DTBNpP.HBF₄ is a **DEVELOPMENTAL** product and is an air-stable form of the free phosphine, which is used as a ligand in metal catalyzed coupling reactions (Suzuki, Heck, Sonogashira, formylations, aminations, and hydrogenations). This reagent is also used in catalytic polymerization reactions. For general reviews of phosphine applications 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.

Product Specification

% Purity by ³¹P NMR

Guaranteed*
95 min

**This product can be made to agreed upon customer specifications*

Solvent None

Physical Properties

Molecular weight	304.0
Density @20°C	>1.0 estimated
Melting point	Not determined to date
Percent volatile	0 %
Pyrophoricity	Non-pyrophoric

Solubility Low in water, soluble in chloroform

Thermal Stability Stable enough to ship and store

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Research / Process Development
Process Validation and Scale Up
Commercial Production



DI-*t*-BUTYLNEOPENTYLPHOSPHONIUM HBF₄ SALT

CAS No. 886059-84-3

OS-PDS-028 Revision: 00

Toxicity/Safety Data Corrosive to eyes (may cause blindness), skin, nose, throat and stomach. May be harmful if swallowed, inhaled, or absorbed through skin.

ADDITIONAL INFORMATION ON SAFETY IS CONTAINED IN THE OPTIMA NEW PRODUCT DATA SHEET (NPDS) AVAILABLE FOR THIS PRODUCT.

Handling/Storage/Disposal Corrosive solid. Do not get in eyes, on skin or clothing. Wash thoroughly after handling. Keep away from heat, sparks and flame. Keep container tightly closed.

Shipping Containers Glass bottle 125 mL, 500 mL

Shipping Limitations Shipments of Di-*tert*-butylneopentylphosphonium tetrafluoroborate are described as "Corrosive solid, acidic, organic, N. O. S. (*DI-T-BUTYL NEOPENTYL PHOSPHINE, TETRAFLUOROBORATE SALT*) 8, UN3261, PGII." Shipments require a "Corrosive" label.

Post, Parcel	Not Acceptable
Sea	Class 8 (IMODG)
Road, Rail	Class 8 (DOT, RID/ADR)
Air	Class 8 (IATA) Cargo Aircraft
	2.5kg max per inner glass containers
	5.0kg max per inner metal containers
	50kg max per outer package

For shipments within Europe, labeling for supply requirements are:

C	Corrosive
R&S Phrase	See New Product 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.