



Tri-*t*-BUTYLPHOSPHINE IN TOLUENE (TTBP)

CAS No. 13716-12-6

QS-PDS-025 Revision: 01

Product Names Tri-*tert*-butylphosphine, Tri-*t*-butylphosphine, TTBP

Formula $[(CH_3)_3C]_3P$

Appearance Colorless to light yellow solution

Application Tri-*t*-butylphosphine (TTBP) solution has been shown to be an excellent ligand for palladium catalyzed Suzuki, Stille and Heck reactions. TTBP is such a powerful ligand that aryl chlorides can be employed as substrates and the reactions can be run at ambient temperatures. For some recent applications, consult: A. F. Littke, C. Dai, and G. C. Fu, *J. Amer. Chem. Soc.*, **2000**, 122, 4020 and S. Lee, M. Jorgensen and J. Hartwig, *Org. Letters*, **2001**, 3, 2729.

Product Specification

	<u>Guaranteed*</u>
TTBP, wt%	5 – 100%
Purity by ³¹ P NMR, %	97 min

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

Solvent Toluene

Physical Properties	
Molecular weight	202.32
Boiling point of pure TTBP	102–103°C at 13 mm
Melting point of pure TTBP	30–31°C
Density @20°C	0.86 g/mL (7.18 lb/gal)
Contained TTBP	108 g/L (0.90 lb/gal)
Flash point	< –30°C
Pyrophoricity	Non-pyrophoric

Solubility In the pure state, TTBP is a low-melting solid. TTBP is very soluble in aliphatic, aromatic and ethereal solvents.

Thermal Stability TTBP is stable at ambient temperature. However, it is very susceptible to oxidation and must be maintained under an inert atmosphere.



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Toxicity/Safety Data Corrosive to the eyes (may cause blindness), skin, mucous membranes and upper respiratory tract. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, motor weakness in fingers and toes, incoordination, and headache. If ingested, may produce a lung aspiration hazard.

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

Handling/Storage/Disposal Use in a closed system under argon or nitrogen. Do not get in eyes, on skin or clothing. Do not breathe vapors or mist. Store in a cool place. Keep container closed. Keep away from sources of ignition, air, acids and oxidizing agents.

Shipping Containers	Bulk containers	2500 – 20000 L
	Cylinders	#5 – 420 L
	Glass bottles	500 mL

Shipping Limitations Shipments of TTBP in toluene are described as "Flammable Liquid, Corrosive, N.O.S., (TRI-TERT-BUTYLPHOSPHINE IN TOLUENE), 3 (8), UN2924, PG II." Shipments require "Flammable Liquid" and "Corrosive" labels.

Post, Parcel	Not acceptable
Sea	Class 3 (8) (IMDG)
Road, Rail (USA)	Class 3 (8) (DOT, RID/ADR)
Air	Class 3 (8) (IATA)
	2.5 L maximum per inner glass container.
	5.0 L maximum per single/outer container.
	Cargo aircraft only.

For shipments within Europe, labeling for supply requirements are:

F	Highly Flammable
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.