



>>Entry Name: Tris(pentafluorophenyl)borane, 9CI

CAS Registry Number: 1109-15-5

$(C_6F_5)_3B$

Molecular Formula: $C_{18}BF_{15}$

Molecular Weight: 511.985

Accurate Mass: 511.98535

Percentage Composition: C 42.23%; B 2.11%; F 55.66%

Source/Synthesis: Synth. from $C_6F_5Li + BCl_3$

Use/Importance: Efficient air-stable and water-tolerant Lewis acid catalyst; catalyst for aldol-type and Michael reactions. Co-catalyst in homogeneous Ziegler-Natta catalysis. Catalyst for polym. of alkenes

Physical Description: Solid

Melting Point: Mp 126-128°

Aldrich: 44259-3

Fluka: 93442

>>Derivative: NH_3 complex

Molecular Formula: $C_{18}H_3BF_{15}N$

Molecular Weight: 529.015

Accurate Mass: 529.011899

Percentage Composition: C 40.87%; H 0.57%; B 2.04%; F 53.87%; N 2.65%

Physical Description: Cryst. ($CHCl_3$)

Melting Point: Mp 178-180°

>>Derivative: Me_3N complex

Molecular Formula: $C_{21}H_9BF_{15}N$

Molecular Weight: 571.096

Accurate Mass: 571.058849

Percentage Composition: C 44.17%; H 1.59%; B 1.89%; F 49.90%; N 2.45%

Physical Description: Cryst. (Et_2O)

Melting Point: Mp 164-166°

>>Derivative: PH_3 complex

Synonym(s): Tris(pentafluorophenyl)(phosphine)boron, 12CI

CAS Registry Number: 132612-63-6

Molecular Formula: $C_{18}H_3BF_{15}P$

Molecular Weight: 545.982

Accurate Mass: 545.982587

Percentage Composition: C 39.60%; H 0.55%; B 1.98%; F 52.20%; P 5.67%

Physical Description: Cryst. (CH_2Cl_2)

References:

- Blaauw, H.J.A. *et al.*, *J. Organomet. Chem.*, 1964, **2**, 245, (synth, ir)
Bradley, D.C. *et al.*, *Chem. Comm.*, 1991, 7, (synth, ir, pmr, cryst struct, PH_3 complex)
Ishihara, K. *et al.*, *Synlett*, 1993, 577, (use)
Brintzinger, H.H. *et al.*, *Angew. Chem., Int. Ed.*, 1995, **34**, 1143-1170, (use, catalysis)
Ishihara, K. *et al.*, *Bull. Chem. Soc. Jpn.*, 1995, **68**, 1721, (use)
Piers, W.E. *et al.*, *Chem. Soc. Rev.*, 1997, **26**, 345-354, (rev)
Chernega, A.N. *et al.*, *J.C.S. Dalton*, 1997, 2293-2303, (synth)