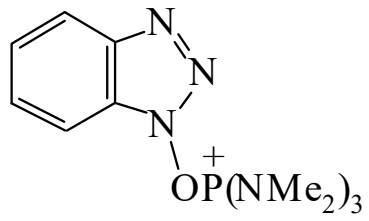
>>**Entry Name: Benzotriazolyloxytris(dimethylamino)phosphonium(1+)**
Synonym(s): (1-Hydroxy-1*H*-benzotriazolato-*O*)tris(*N*-methylmethanaminato)phosphorus(1+), 9Cl. (1-Hydroxy-1*H*-benzotriazolato-*O*)tris(dimethylamino)phosphorus(1+). Castro reagent. Le BOP reagent



Molecular Formula: $C_{12}H_{22}N_6OP^{(+)}$
Molecular Weight: 297.319
Accurate Mass: 297.159271
Percentage Composition: C 48.48%; H 7.46%; N 28.27%; O 5.38%; P 10.42%

>>**Derivative:** Chloride
Synonym(s): BOP

CAS Registry Number: 62157-09-9

Molecular Formula: $C_{12}H_{22}ClN_6OP$
Molecular Weight: 332.772
Accurate Mass: 332.128123
Percentage Composition: C 43.31%; H 6.66%; Cl 10.65%; N 25.25%; O 4.81%; P 9.31%
Physical Description: No phys. props. reported

>>**Derivative:** Tetrafluoroborate

Molecular Formula: $C_{12}H_{22}BF_4N_6OP$
Molecular Weight: 384.124
Accurate Mass: 384.162188
Percentage Composition: C 37.52%; H 5.77%; B 2.81%; F 19.78%; N 21.88%; O 4.17%; P 8.06%
Physical Description: Cryst. (MeCN/petrol)
Melting Point: Mp 129-131°

>>**Derivative:** Hexafluorophosphate

CAS Registry Number: 56602-33-6

Molecular Formula: $C_{12}H_{22}F_6N_6OP_2$
Molecular Weight: 442.283
Accurate Mass: 442.123451
Percentage Composition: C 32.59%; H 5.01%; F 25.77%; N 19.00%; O 3.62%; P 14.01%
Use/Importance: Coupling agent for peptides (sometimes in conjunction with Hexakis(dimethylamino)-μ-oxodiphosphorus(2+) CKV07-T) and also nucleotides; and for esterification of carboxylic acids by phenols. Allows selective esterification in carbohydrates
Physical Description: Cryst. (Me_2CO/Et_2O)
Melting Point: Mp 147-149°
Other Data: Shown to be superior overall as a peptide coupling reagent to 3 other reagents commonly employed (Dudash *et al*)
Aldrich: 22608-4
Fluka: 12802
Sigma: B2886

References:

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Castro, B. *et al.*, *Synthesis*, 1976, 751; 1977, 413, *(synth, pmr, nmr, ir, use)*
Galpin, I.J. *et al.*, *Tetrahedron*, 1976, **32**, 2417, *(use)*
Glass, R.S. *et al.*, *Tet. Lett.*, 1979, 3321, *(synth, use)*
Chapleur, Y. *et al.*, *J.C.S. Perkin 1*, 1980, 1940; 2683, *(use)*
Appel, R. *et al.*, *Chem. Ber.*, 1981, **114**, 2649, *(use)*
Dudash, J. *et al.*, *Synth. Commun.*, 1993, **23**, 349