



>>Entry Name: Trioctylphosphine, 9CI

CAS Registry Number: 4731-53-7

Related CAS Registry Numbers(s): 56022-37-8

$\text{P}[(\text{CH}_2)_7\text{CH}_3]_3$

Molecular Formula: $\text{C}_{24}\text{H}_{51}\text{P}$

Molecular Weight: 370.641

Accurate Mass: 370.372837

Percentage Composition: C 77.77%; H 13.87%; P 8.36%

Use/Importance: Metal extractant. Exhibits synergistic activity with other extractants. Extracts mineral acids (HCl, HBr, HNO_3 , H_2SO_4 , HClO_4) from aq. soln. Used in catalysts for prep. of polymers, and for the dimerization of alkenes

Melting Point: Mp 30°. Mp 48°

Boiling Point: Bp₁ 194-195°. Bp 234°

Refractive Index: n_D^{25} 1.4666

Aldrich: 11785-4

Fluka: 92840

Rare Chemicals Library: S44065-5

>>Derivative: Methiodide

Synonym(s): Methyltrioctylphosphonium iodide

Molecular Formula: $\text{C}_{25}\text{H}_{54}\text{IP}$

Molecular Weight: 512.58

Accurate Mass: 512.300785

Percentage Composition: C 58.58%; H 10.62%; I 24.76%; P 6.04%

Physical Description: Liq.

>>Derivative: Oxide

Synonym(s): Trioctylphosphine oxide, 9CI. TOPO

CAS Registry Number: 78-50-2

Molecular Formula: $\text{C}_{24}\text{H}_{51}\text{OP}$

Molecular Weight: 386.64

Accurate Mass: 386.367752

Percentage Composition: C 74.56%; H 13.29%; O 4.14%; P 8.01%

Use/Importance: Extracts carboxylic acids from aq. solns. Widely used as a metal extractant, particularly for rare earth metals, and in the chromatography of these.

Employed in catalysts for the cyclotrimerization of butadiene and for the cross-linking of epoxy resins

Physical Description: Cryst. (cyclohexane)

Melting Point: Mp 49-50°. Mp 59.5-60°

Boiling Point: Bp₃ 225-228°

Solubility: Sol. cyclohexanone (35.6g per 100 cm³, 25°), common org. solvs.

pKa Value: $\text{p}K_{\text{a1}}$ 8.8 (MeNO_2)

Aldrich: 34618-7

Fluka: 92850

Sigma: T4760

>>Derivative: Sulfide

CAS Registry Number: 2551-53-3

Molecular Formula: $\text{C}_{24}\text{H}_{51}\text{PS}$

Molecular Weight: 402.707

Accurate Mass: 402.344907

Percentage Composition: C 71.58%; H 12.76%; P 7.69%; S 7.96%

Use/Importance: Selective metal extractant. Possesses bactericidal and fungicidal activity

Physical Description: Liq.

Boiling Point: Bp₁ 226-228°

References: