



>>Variant: (±)-form

**Molecular Formula:** C<sub>7</sub>H<sub>9</sub>O<sub>3</sub>P

**Molecular Weight:** 172.12

**Accurate Mass:** 172.028932

**Percentage Composition:** C 48.85%; H 5.27%; O 27.89%; P 18.00%

**Physical Description:** Oil

**pKa Value:** pK<sub>a</sub> 2.97

**Other Data:** Heat-sensitive, isol. as Ba or cyclohexylammonium salt

>>Derivative: Mono-cyclohexylammonium salt

**CAS Registry Number:** 38555-73-6

**Physical Description:** Cryst. (Me<sub>2</sub>CO)

**Melting Point:** Mp 156-158°

>>Derivative: Mono-dicyclohexylammonium salt

**CAS Registry Number:** 75620-16-5

**Physical Description:** Cryst. (hexane)

**Melting Point:** Mp 132°

>>Derivative: Me ester

>>Derivative: (4-Bromo-2,5-dichlorophenyl) ester

**Synonym(s):** (4-Bromo-2,5-dichlorophenyl)methyl phenylphosphonate. Leptophos Oxon

**CAS Registry Number:** 25006-32-0

**Molecular Formula:** C<sub>13</sub>H<sub>10</sub>BrCl<sub>2</sub>O<sub>3</sub>P

**Molecular Weight:** 396.003

**Accurate Mass:** 393.912797

**Percentage Composition:** C 39.43%; H 2.55%; Br 20.18%; Cl 17.91%; O 12.12%; P 7.82%

**Use/Importance:** Metab. of, and a more powerful neurotoxic agent than, Leptophos

>>Derivative: Chloride

#### References:

- Cherbuliez, E. *et al.*, *Helv. Chim. Acta*, 1961, **44**, 1812, (*synth*)  
Holmstead, R.L. *et al.*, *Arch. Environ. Contam. Toxicol.*, 1973, **1**, 133; *CA*, **80**, 44526, (*ms*)  
Brooks, R.J. *et al.*, *J.O.C.*, 1973, **38**, 1614, (*synth, pmr*)  
Lee, P.W. *et al.*, *Arch. Environ. Contam. Toxicol.*, 1976, **4**, 443; *CA*, **86**, 66794, (*deriv*)  
Felcht, U. *et al.*, *Chem. Ber.*, 1976, **109**, 3675, (*synth, ir*)  
Otsuki, T. *et al.*, *Synthesis*, 1981, 811, (*ester*)  
Regitz, M. *et al.*, *Annalen*, 1984, 1641, (*pmr*)  
Morgan, B.P. *et al.*, *J.A.C.S.*, 1991, **113**, 297, (*synth, uv, pmr, cmr, P-31 nmr*)  
Baker, S.M. *et al.*, *J. Agric. Food Chem.*, 1995, **43**, 503-506, (*Leptophos oxon, cryst struct*)