



>>Variant: (±)-form

Molecular Formula: C₇H₉O₃P

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_a 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. (Me₂CO)

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: C₁₃H₁₀BrCl₂O₃P

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*)