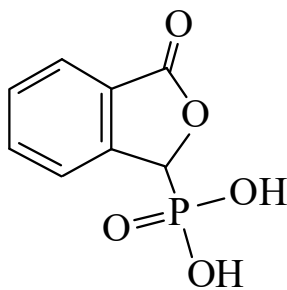




>>Entry Name: (1,3-Dihydro-3-oxo-1-isobenzofuranyl)phosphonic acid, 9Cl

Synonym(s): Phthalide-3-phosphonic acid. 3-Phosphonophthalide



CAS Registry Number: 4741-67-7

Related CAS Registry Numbers(s): 130284-16-1 130284-21-8

Molecular Formula: C₈H₇O₅P

Molecular Weight: 214.114

Accurate Mass: 214.003112

Percentage Composition: C 44.88%; H 3.30%; O 37.36%; P 14.47%

Physical Description: Needles + 1H₂O (H₂O)

Melting Point: Mp 253-254°

>>Derivative: Mono-Me ester

Molecular Formula: C₉H₉O₅P

Molecular Weight: 228.141

Accurate Mass: 228.018762

Percentage Composition: C 47.38%; H 3.98%; O 35.06%; P 13.58%

Physical Description: Cryst. (CH₂Cl₂/Et₂O)

Melting Point: Mp 176°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl (1,3-dihydro-3-oxo-1-isobenzofuranyl)phosphonate

CAS Registry Number: 61260-15-9

Molecular Formula: C₁₀H₁₁O₅P

Molecular Weight: 242.168

Accurate Mass: 242.034412

Percentage Composition: C 49.60%; H 4.58%; O 33.03%; P 12.79%

Physical Description: Cryst. (C₆H₆/cyclohexane)

Melting Point: Mp 96-97°

>>Derivative: Diisopropyl ester

Synonym(s): Diisopropyl (1,3-dihydro-3-oxo-1-isobenzofuranyl)phosphonate

Molecular Formula: C₁₄H₁₉O₅P

Molecular Weight: 298.275

Accurate Mass: 298.097012

Percentage Composition: C 56.38%; H 6.42%; O 26.82%; P 10.38%

Physical Description: Cryst. (C₆H₆/cyclohexane)

Melting Point: Mp 98-99°

References:

- Ramirez, F. *et al.*, *J.A.C.S.*, 1961, **83**, 173, (*synth, esters, ir, struct*)
Napolitano, E. *et al.*, *Synthesis*, 1985, 38, (*di-Me ester, ir, pmr, use*)
Stowell, M.H.B. *et al.*, *Tet. Lett.*, 1990, **31**, 3261, (*dichloride, ms, P-31 nmr*)
Janowski, W.K. *et al.*, *Aust. J. Chem.*, 1991, **44**, 477, (*synth, mono-Me ester, ir, pmr*)