



>>Entry Name: (2-Oxo-4-phenylbutyl)phosphonic acid, 9CI

CAS Registry Number: 51008-95-8

PhCH2CH2COCH2P(O)(OH)2

Molecular Formula: C₁₀H₁₃O₄P

Molecular Weight: 228.184

Accurate Mass: 228.055147

Percentage Composition: C 52.64%; H 5.74%; O 28.05%; P 13.57%

Use/Importance: Esters are reagents widely employed in prostaglandin synth., and in the synth. of αβ-cyclohexenones

Physical Description: Solid

Melting Point: Mp 153-154°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl (2-oxo-4-phenylbutyl)phosphonate

CAS Registry Number: 41162-19-0

Molecular Formula: C₁₂H₁₇O₄P

Molecular Weight: 256.238

Accurate Mass: 256.086447

Percentage Composition: C 56.25%; H 6.69%; O 24.98%; P 12.09%

Use/Importance: Used in cyclohexenone synth.

Physical Description: Liq.

Boiling Point: Bp_{0.5} 120-122°

>>Derivative: Di-Et ester

Synonym(s): Diethyl (2-oxo-4-phenylbutyl)phosphonate

CAS Registry Number: 40601-45-4

Molecular Formula: C₁₄H₂₁O₄P

Molecular Weight: 284.291

Accurate Mass: 284.117747

Percentage Composition: C 59.15%; H 7.45%; O 22.51%; P 10.90%

Physical Description: Liq.

Boiling Point: Bp_{0.12} 162°

Refractive Index: n_D¹⁵ 1.5060

References:

Göhring, G. *et al.*, *Chem. Ber.*, 1973, **106**, 2460, (*synth, ester, ir, pmr, ms*)

Grieco, P.A. *et al.*, *J.A.C.S.*, 1973, **95**, 3071, (*ester*)

Chattha, M. *et al.*, *J.O.C.*, 1973, **38**, 2908, (*ester*)

Grieco, P.A. *et al.*, *Synthesis*, 1973, 425, (*use*)

Magerlein, B.J. *et al.*, *Prostaglandins*, 1975, **9**, 5, (*use*)

De Jongh, C.P. *et al.*, *Heteroat. Chem.*, 1990, **1**, 503, (*diethyl ester, ir, ms, pmr, cmr, P-31 nmr*)