



>>Entry Name: Methylphosphonic acid, 9CI

Synonym(s): Methanephosphonic acid

CAS Registry Number: 993-13-5

MeP(O)(OH)<sub>2</sub>

Molecular Formula: CH<sub>5</sub>O<sub>3</sub>P

Molecular Weight: 96.022

Accurate Mass: 95.997632

Percentage Composition: C 12.51%; H 5.25%; O 49.99%; P 32.26%

Physical Description: Hygroscopic cryst.

Melting Point: Mp 105°

Solubility: Sol. H<sub>2</sub>O, EtOH, Et<sub>2</sub>O

pKa Value: pK<sub>a1</sub> 2.41; pK<sub>a2</sub> 7.35 (25°) pK<sub>a1</sub> 2.38; pK<sub>a2</sub> 7.74 (25°,H<sub>2</sub>O)

Hazard & Toxicity: Highly irritant. Corrosive

Aldrich: 28986-8

Fluka: 64259

>>Derivative: Anilinium salt

Physical Description: Cryst. (propanol)

Melting Point: Mp 149-150°

>>Derivative: Mono-Me ester

>>Derivative: Di-Me ester

>>Derivative: Mono-Et ester

>>Derivative: Di-Et ester

>>Derivative: Monopropyl ester

Synonym(s): Propyl hydrogen methylphosphonate

CAS Registry Number: 4546-11-6

Molecular Formula: C<sub>4</sub>H<sub>11</sub>O<sub>3</sub>P

Molecular Weight: 138.103

Accurate Mass: 138.044582

Percentage Composition: C 34.79%; H 8.03%; O 34.76%; P 22.43%

Physical Description: Liq.

Boiling Point: Bp<sub>0.05</sub> 106°

Refractive Index: n<sub>D</sub><sup>25</sup> 1.4259

>>Derivative: Dipropyl ester

Synonym(s): Dipropyl methylphosphonate

CAS Registry Number: 6410-56-6

Molecular Formula: C<sub>7</sub>H<sub>17</sub>O<sub>3</sub>P

Molecular Weight: 180.183

Accurate Mass: 180.091532

Percentage Composition: C 46.66%; H 9.51%; O 26.64%; P 17.19%

Physical Description: Liq.

Boiling Point: Bp<sub>9</sub> 93-96°. Bp<sub>0.25</sub> 115.5°

Density: d<sub>4</sub><sup>20</sup> 1.01

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4210