



>>Entry Name: (Cyanomethyl)phosphonic acid, 9CI

CAS Registry Number: 35236-60-3

Related CAS Registry Numbers(s): 25117-54-8 67393-39-9 67393-40-2 73639-51-7

NCCH<sub>2</sub>P(O)(OH)<sub>2</sub>

Molecular Formula: C<sub>2</sub>H<sub>4</sub>NO<sub>3</sub>P

Molecular Weight: 121.032

Accurate Mass: 120.992881

Percentage Composition: C 19.85%; H 3.33%; N 11.57%; O 39.66%; P 25.59%

>>Derivative: Mono-anilinium salt

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

Melting Point: Mp 172-174 dec.°

>>Derivative: Di-Et ester

Synonym(s): Diethyl (cyanomethyl)phosphonate

CAS Registry Number: 2537-48-6

Molecular Formula: C<sub>6</sub>H<sub>12</sub>NO<sub>3</sub>P

Molecular Weight: 177.139

Accurate Mass: 177.055481

Percentage Composition: C 40.68%; H 6.83%; N 7.91%; O 27.10%; P 17.49%

Use/Importance: Wittig-Horner reagent for synth. of acrylonitriles (1-cyanoethenes)

Physical Description: Liq.

Boiling Point: Bp<sub>0.02</sub> 88-94°

Aldrich: D9170-5

Fluka: 28503

Sigma: D6640

>>Derivative: Diisopropyl ester

Synonym(s): Diisopropyl (cyanomethyl)phosphonate. Diisopropylphosphonoacetonitrile

CAS Registry Number: 21658-95-7

Extra CAS Registry Numbers(s): 58264-04-3

Molecular Formula: C<sub>8</sub>H<sub>16</sub>NO<sub>3</sub>P

Molecular Weight: 205.193

Accurate Mass: 205.086781

Percentage Composition: C 46.83%; H 7.86%; N 6.83%; O 23.39%; P 15.09%

Use/Importance: Reagent used in the preparation of retinoids and carotenoids

Boiling Point: Bp<sub>0.5</sub> 126-128°. Bp<sub>0.08</sub> 108-110°

Density: d<sub>4</sub><sup>20</sup> 1.05

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4288

>>Derivative: Bis(trimethylsilyl) ester

Synonym(s): Bis(trimethylsilyl) (cyanomethyl)phosphonate

Molecular Formula: C<sub>8</sub>H<sub>20</sub>NO<sub>3</sub>PSi<sub>2</sub>

Molecular Weight: 265.396

Accurate Mass: 265.071935

Percentage Composition: C 36.21%; H 7.60%; N 5.28%; O 18.09%; P 11.67%; Si 21.17%

Physical Description: Liq.

Boiling Point: Bp<sub>7</sub> 129-130°

>>Derivative: Diamide, *N,N,N',N'*-tetra-Me

Synonym(s): (Cyanomethyl)phosphonic bis(dimethylamide). *P*-(Cyanomethyl)-*N,N,N',N'*-tetramethylphosphonic diamide

Molecular Formula: C<sub>6</sub>H<sub>14</sub>N<sub>3</sub>OP

Molecular Weight: 175.17

Accurate Mass: 175.087449

Percentage Composition: C 41.14%; H 8.06%; N 23.99%; O 9.13%; P 17.68%

Physical Description: Cryst. (Et<sub>2</sub>O/dimethoxyethane)

Melting Point: Mp 93°

References: