



>>Entry Name: Phorate, BSI

Synonym(s): *O,O*-Diethyl *S*-[(ethylthio)methyl] phosphorodithioate, 9CI. Thimet. Granutox

CAS Registry Number: 298-02-2

(EtO)₂P(S)SCH₂SEt

Molecular Formula: C₇H₁₇O₂PS₃

Molecular Weight: 260.382

Accurate Mass: 260.012827

Percentage Composition: C 32.29%; H 6.58%; O 12.29%; P 11.90%; S 36.94%

Use/Importance: Insecticide, acaricide

Physical Description: Mobile liq.

Boiling Point: Bp_{0.8} 118-120°

Density: d₄²⁵ 1.167

Refractive Index: n_D²⁵ 1.5349

Other Data: Metab. *via* the sulfoxide and sulfone

Hazard & Toxicity: Very toxic if swallowed or in contact with skin. LD₅₀ (rat, orl) 1 mg/kg, LC₅₀ (rat, ihl) 11 mg/m⁻³ (1h exposure), LD₅₀ (rat, skn) 2.5 mg/kg. Cholinesterase inhibitor. Readily adsorbed by skin. OES: long-term 0.05 ppm; short-term 0.2 ppm (Sk)

Supelco: R60-0365

>>Derivative: *S*-Oxide

Synonym(s): *O,O*-Diethyl *S*-[(ethylsulfinyl)methyl] phosphorodithioate

CAS Registry Number: 2588-03-6

Molecular Formula: C₇H₁₇O₃PS₃

Molecular Weight: 276.381

Accurate Mass: 276.007742

Percentage Composition: C 30.42%; H 6.20%; O 17.37%; P 11.21%; S 34.81%

Use/Importance: Metabolite of phorate

Physical Description: Liq.

Boiling Point: Bp_{0.1} 150°

Density: d₄²⁵ 1.23

Refractive Index: n_D³⁰ 1.5365

Hazard & Toxicity: LD₅₀ (rat, orl) 2 mg/kg

>>Derivative: *S,S*-Dioxide

Synonym(s): *O,O*-Diethyl *S*-[(ethylsulfonyl)methyl] phosphorodithioate

CAS Registry Number: 2588-04-7

Molecular Formula: C₇H₁₇O₄PS₃

Molecular Weight: 292.381

Accurate Mass: 292.002657

Percentage Composition: C 28.76%; H 5.86%; O 21.89%; P 10.59%; S 32.90%

Use/Importance: Metabolite of phorate

Physical Description: Liq.

Boiling Point: Bp_{0.1} 150°

Density: d₄²⁵ 1.26

Refractive Index: n_D³⁰ 1.5251

Hazard & Toxicity: LD₅₀ (rat, orl) 1.7 mg/kg

References: