



>>Derivative: Me ester

CAS Registry Number: 35909-92-3

Molecular Formula: C₁₈H₁₉NO₄

Molecular Weight: 313.352

Accurate Mass: 313.131409

Percentage Composition: C 69.00%; H 6.11%; N 4.47%; O 20.42%

Physical Description: Oil

Optical Rotation: [α]_D −16 (c, 1.6 in MeOH)

>>Derivative: 4-Nitrophenyl ester

CAS Registry Number: 2578-84-9

Molecular Formula: C₂₃H₂₀N₂O₆

Molecular Weight: 420.421

Accurate Mass: 420.132138

Percentage Composition: C 65.71%; H 4.79%; N 6.66%; O 22.83%

Melting Point: Mp 126.5-127.5°

Optical Rotation: [α]_D −8.9 (c, 2.2 in EtOAc)

Sigma: C4627

>>Derivative: 2,4,5-Trichlorophenyl ester

CAS Registry Number: 3065-27-8

Molecular Formula: C₂₃H₁₈Cl₃NO₄

Molecular Weight: 478.758

Accurate Mass: 477.03014

Percentage Composition: C 57.70%; H 3.79%; Cl 22.22%; N 2.93%; O 13.37%

Melting Point: Mp 140-141°

Optical Rotation: [α]_D −40.1 (c, 1 in DMF)

>>Derivative: Pentachlorophenyl ester

CAS Registry Number: 3086-21-3

Molecular Formula: C₂₃H₁₆Cl₅NO₄

Molecular Weight: 547.647

Accurate Mass: 544.952194

Percentage Composition: C 50.44%; H 2.94%; Cl 32.37%; N 2.56%; O 11.69%

Melting Point: Mp 154-155°

Optical Rotation: [α]_D −49.5 (c, 1 in DMF)

>>Derivative: Succinimido ester

CAS Registry Number: 3397-32-8

Molecular Formula: C₂₁H₂₀N₂O₆

Molecular Weight: 396.399

Accurate Mass: 396.132138

Percentage Composition: C 63.63%; H 5.09%; N 7.07%; O 24.22%

Melting Point: Mp 140-140.5°

Optical Rotation: [α]_D²⁵ −17.3 (c, 2 in dioxan)

>>Derivative: Amide

Synonym(s): Z-PheNH₂

CAS Registry Number: 4801-80-3

Molecular Formula: C₁₇H₁₈N₂O₃

Molecular Weight: 298.341

Accurate Mass: 298.131743

Percentage Composition: C 68.44%; H 6.08%; N 9.39%; O 16.09%

Melting Point: Mp 164-165°

Optical Rotation: [α]_D −6.8 (c, 1 in MeOH)