



>>Derivative: *N*-2,4-Dinitrophenyl

CAS Registry Number: 1655-54-5

Molecular Formula: C₁₅H₁₃N₃O₆

Molecular Weight: 331.284

Accurate Mass: 331.080437

Percentage Composition: C 54.38%; H 3.96%; N 12.68%; O 28.98%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 189°

Sigma: D1380

>>Derivative: 4-Nitroanilide, *N*-Ac

CAS Registry Number: 17682-83-6

Molecular Formula: C₁₇H₁₇N₃O₄

Molecular Weight: 327.339

Accurate Mass: 327.121907

Percentage Composition: C 62.38%; H 5.23%; N 12.84%; O 19.55%

Melting Point: Mp 244-246°

Optical Rotation: [α]_D²⁰ +97.9 (MeOH)

>>Variant: (±)-form

Synonym(s): FEMA 3726

CAS Registry Number: 150-30-1

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Prisms (H₂O)

Melting Point: Mp 271-273°. Mp 284-288 dec., 318-320° dec.°

Solubility: Spar. sol. H₂O, EtOH; insol. Et₂O

pKa Value: pK_{a1} 2.16; pK_{a2} 9.15 (25°, NH₃⁽⁺⁾, 0.1M NaCl)

Aldrich: 14796-6

Fluka: 78040

Sigma: P1876

>>Derivative: Hydrochloride

CAS Registry Number: 27172-85-6

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 234-235°

>>Derivative: Me ester

CAS Registry Number: 15028-44-1

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Liq.

Boiling Point: Bp₁₂ 141°

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 5619-07-8

Physical Description: Needles

Melting Point: Mp 158 dec.°

Sigma: P3001