



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

CAS Registry Number: 1694-97-9

Melting Point: Mp 132°

Sigma: D2380

>>Variant: (±)-form

Synonym(s): FEMA 3444

CAS Registry Number: 516-06-3

Molecular Formula: C₅H₁₁NO₂

Molecular Weight: 117.147

Accurate Mass: 117.078979

Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%

Use/Importance: Flavouring ingredient

Physical Description: Plates (EtOH)

Melting Point: Mp 298 dec.° (sealed tube)

Solubility: Sol. H₂O; insol. EtOH, Et₂O

pKa Value: p*K*_{a1} 2.35; p*K*_{a2} 9.62 (25°)

Other Data: Sublimes

Aldrich: W34440-0

Fluka: 94640

Sigma: V6379

>>Derivative: Hydrochloride

CAS Registry Number: 25616-14-2

Physical Description: Cryst. (hot H₂O), leaflets (dil. HCl)

Melting Point: Mp 189°

>>Derivative: Me ester

CAS Registry Number: 5619-05-6

Physical Description: Plates (MeOH/Et₂O)

Melting Point: Mp 120-122° (as hydrochloride)

Sigma: V0875

>>Derivative: Et ester

CAS Registry Number: 13893-45-3

Physical Description: Liq.

Boiling Point: Bp 174° part. dec.. Bp₈ 63.5°

Solubility: V. sol. H₂O

Density: d¹⁵ 0.9617

>>Derivative: Et ester; hydrochloride

CAS Registry Number: 23358-42-1

Physical Description: Hygroscopic cryst.

Melting Point: Mp 76°

>>Derivative: Et ester, picrate

Physical Description: Cryst.

Melting Point: Mp 139.5°

>>Derivative: Butyl ester

CAS Registry Number: 110470-28-5

Physical Description: Syrup

Boiling Point: Bp₁₇ 98-98.5°

Solubility: Sol. H₂O, EtOH, Et₂O, CHCl₃

Density: d¹⁴ 0.9266