



CAS Registry Number: 134-20-3

Molecular Formula: $C_8H_9NO_2$

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Biological Source: Found in essential oils, including bergamot, orange peel, lemon peel, jasmine, ylang-ylang and neroli. Also present in concord grape, strawberry, star fruit, wines, cocoa, black tea and rice bran

Use/Importance: Used in perfumery as artificial orange blossom fragrance, also employed extensively in the form of its Schiff's bases (e.g. with Hydroxycitronellal). Flavouring agent

Physical Description: Cryst.

Melting Point: Mp 24-25°

Boiling Point: Bp₁₅ 133.5°

pKa Value: pK_a 2.32 (25°, 1% EtOH aq.)

Other Data: Steam-volatile

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2910 mg/kg. Exp. reprod. effects

Aldrich: 23645-4

Fluka: 10730

Sigma: M3888

>> **Derivative:** Et ester

Synonym(s): FEMA 2421

CAS Registry Number: 87-25-2

Molecular Formula: $C_9H_{11}NO_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

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

Physical Description: Liq. with feint orang-flower odour and flavour

Melting Point: Mp 13°

Boiling Point: Bp 266-268°. Bp₁₅ 145-147°

Density: d₄²⁰ 1.117

Aldrich: 24297-7

Fluka: 10700