



CAS Registry Number: 6982-39-4
Molecular Formula: C₆H₁₃NO
Molecular Weight: 115.175
Accurate Mass: 115.099714
Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%
Melting Point: Mp 68°
Boiling Point: Bp₁₅ 108-110°
pKa Value: pK_a 9.63

>>Derivative: Hydrochloride

CAS Registry Number: 5456-63-3
Melting Point: Mp 175°
Aldrich: 22257-7

>>Derivative: *O*-Benzoyl

Molecular Formula: C₁₃H₁₇NO₂
Molecular Weight: 219.283
Accurate Mass: 219.125929
Percentage Composition: C 71.21%; H 7.81%; N 6.39%; O 14.59%
Physical Description: Needles (EtOH) (as hydrochloride)
Melting Point: Mp 274° (hydrochloride)

>>Variant: (1*RS*,2*SR*)-form
Synonym(s): (±)-*cis*-form

CAS Registry Number: 931-15-7
Molecular Formula: C₆H₁₃NO
Molecular Weight: 115.175
Accurate Mass: 115.099714
Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%
Melting Point: Mp 107-108°
Boiling Point: Bp₁₅ 108-110°
pKa Value: pK_a 9.72

>>Derivative: Hydrochloride

Physical Description: Cryst. (EtOH/Et₂O)
Melting Point: Mp 188-189°

>>Derivative: *O*-Benzoyl

Molecular Formula: C₁₃H₁₇NO₂
Molecular Weight: 219.283
Accurate Mass: 219.125929
Percentage Composition: C 71.21%; H 7.81%; N 6.39%; O 14.59%
Physical Description: Needles (EtOH/Et₂O) (as hydrochloride)
Melting Point: Mp 228° (hydrochloride)

References:

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Ursini, A. *et al.*, *Synth. Commun.*, 1999, **29**, 1369-1377, (1*S*,2*S*-form, *resoln*, *pmr*)