



>>Variant: (2*RS*,3*RS*)-form

Synonym(s): (±)-Allothreonine

CAS Registry Number: 144-98-9

Molecular Formula: C₄H₉NO₃

Molecular Weight: 119.12

Accurate Mass: 119.058244

Percentage Composition: C 40.33%; H 7.62%; N 11.76%; O 40.29%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 273-274° (269-270° dec.)

Other Data: Crystallises as a conglomerate resolvable by crystallisation

Sigma: T9643

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 76419-75-5

Melting Point: Mp 150 dec.°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₁H₁₃NO₄

Molecular Weight: 223.228

Accurate Mass: 223.084459

Percentage Composition: C 59.19%; H 5.87%; N 6.27%; O 28.67%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 175-176°

>>Derivative: Me ether

Molecular Formula: C₅H₁₁NO₃

Molecular Weight: 133.147

Accurate Mass: 133.073894

Percentage Composition: C 45.10%; H 8.33%; N 10.52%; O 36.05%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 230-233°

>>Variant: (2*RS*,3*SR*)-form

Synonym(s): (±)-Threonine

CAS Registry Number: 80-68-2

Molecular Formula: C₄H₉NO₃

Molecular Weight: 119.12

Accurate Mass: 119.058244

Percentage Composition: C 40.33%; H 7.62%; N 11.76%; O 40.29%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 234-235 dec.°

Aldrich: T3422-3

Fluka: 89200

Sigma: T1520

>>Derivative: Me ester

CAS Registry Number: 53216-06-1

Molecular Formula: C₅H₁₁NO₃

Molecular Weight: 133.147

Accurate Mass: 133.073894

Percentage Composition: C 45.10%; H 8.33%; N 10.52%; O 36.05%

Melting Point: Mp 125 dec.° (as hydrochloride)

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₁H₁₃NO₄

Molecular Weight: 223.228

Accurate Mass: 223.084459

Percentage Composition: C 59.19%; H 5.87%; N 6.27%; O 28.67%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 143-144°