



Molecular Weight: 180.16
Accurate Mass: 180.04226
Percentage Composition: C 60.00%; H 4.48%; O 35.52%

>>Derivative: Me ether

Melting Point: Mp 261-264 dec.° (as K salt)

>>Derivative: Me ether, Me ester

CAS Registry Number: 42245-42-1
Molecular Formula: C₁₁H₁₂O₄
Molecular Weight: 208.213
Accurate Mass: 208.07356
Percentage Composition: C 63.45%; H 5.81%; O 30.74%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 66-69°
Boiling Point: Bp₄₀ 104-106°
Aldrich: 29798-4

>>Derivative: Me ether, Et ester

Physical Description: Yellow cryst. (EtOH)
Melting Point: Mp 40-43°
Boiling Point: Bp_{1.5} 154-156°

>>Derivative: Me ether, amide

Molecular Formula: C₁₀H₁₁NO₃
Molecular Weight: 193.202
Accurate Mass: 193.073894
Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 151°

>>Derivative: Me ether, nitrile

Molecular Formula: C₁₀H₉NO₂
Molecular Weight: 175.187
Accurate Mass: 175.063329
Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%
Boiling Point: Bp₆ 156-157°
Density: d₄²⁵ 1.17
Refractive Index: n_D²⁰ 1.5500

References:

- Roux-Schmitt, M.C., *Tetrahedron*, 1972, **28**, 4965, (*pmr*)
Cragg, J.E. *et al.*, *J.C.S. Perkin I*, 1982, 2487, (*synth, ir, pmr, ms*)
Crotti, P. *et al.*, *J.O.C.*, 1986, **51**, 2759, (*synth, derivs, pmr*)
Svoboda, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1988, **53**, 822, (*synth, derivs, pmr, ms*)
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Watson, K.G. *et al.*, *Chem. Comm.*, 1990, 1018, (*synth, derivs, resoln*)
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