



Physical Description: Needles
Melting Point: Mp 117°
Optical Rotation: $[\alpha]_{\text{Hg}}^{20} -20.1$ (Py)

>>**Derivative:** *N*-(2,4,6-Trimethylbenzenesulfonyl)

CAS Registry Number: 139192-50-0
Molecular Formula: C₁₄H₂₃NO₃S
Molecular Weight: 285.407
Accurate Mass: 285.139864
Percentage Composition: C 58.92%; H 8.12%; N 4.91%; O 16.82%; S 11.24%
Physical Description: Cryst. (hexane/Et₂O)
Melting Point: Mp 71°
Optical Rotation: $[\alpha]_{\text{D}}^{20} -37.8$ (c, 1.13 in CHCl₃)

>>**Variant:** (±)-form

CAS Registry Number: 16369-05-4
Molecular Formula: C₅H₁₃NO
Molecular Weight: 103.164
Accurate Mass: 103.099714
Percentage Composition: C 58.21%; H 12.70%; N 13.58%; O 15.51%
Physical Description: Oil
Boiling Point: Bp 181-186°. Bp₁₀ 95-100°
Solubility: Sol. H₂O, EtOH; mod. sol. Et₂O
Other Data: Spar. steam-volatile
Sigma: V4002

>>**Derivative:** Hydrochloride

Physical Description: Plates (Me₂CO)
Melting Point: Mp 118-119°

>>**Derivative:** Dibenzoyl

Physical Description: Prisms (Me₂CO aq.)
Melting Point: Mp 114°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 336C; 336D, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 540B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 426A; 426B; 426C, (*ir*)
Karrer, P. *et al.*, *Helv. Chim. Acta*, 1922, **5**, 478; 1949, **32**, 1156, (*synth, abs config*)
Barrow, F. *et al.*, *J.C.S.*, 1935, 410, (*synth, abs config*)
Kurth, M.J. *et al.*, *J.A.C.S.*, 1985, **107**, 443, (*use*)
Meyers, A.I. *et al.*, *Tet. Lett.*, 1985, **26**, 2047, (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1986, **12**, 563; 1988, **13**, 341; **16**, 380, (*use*)
Ibuka, T. *et al.*, *J.O.C.*, 1997, **62**, 999-1015, (2,4,6-trimethylbenzenesulfonyl, *synth, pmr*)
Segat-Dioury, F. *et al.*, *Tetrahedron*, 2000, **56**, 233-248, (*S-form, synth*)