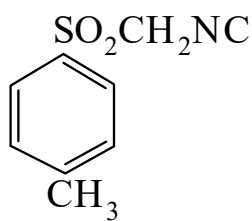




>>Entry Name: Isocyanomethyl 4-methylphenyl sulfone

Synonym(s): 1-[(Isocyanomethyl)sulfonyl]-4-methylbenzene, 9CI. Isocyanomethyl *p*-tolyl sulfone. *p*-Tolylsulfonylmethyl isocyanide. Tosylmethyl isocyanide. TosMIC



CAS Registry Number: 36635-61-7

Molecular Formula: C₉H₉NO₂S

Molecular Weight: 195.242

Accurate Mass: 195.035399

Percentage Composition: C 55.37%; H 4.65%; N 7.17%; O 16.39%; S 16.42%

Use/Importance: Reagent for homologation of carboxylic acids and used in synth. of 1,5 and 1,6-diketones

Physical Description: Cryst. (C₆H₆/cyclohexane)

Melting Point: Mp 114-115° (110°)

Other Data: α-Substd. analogues are also versatile reagents

Aldrich: 18820-4

Fluka: 89816

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 808B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 487A, (*ir*)

Schöllkopf, U. *et al.*, *Angew. Chem., Int. Ed.*, 1972, **11**, 311, (*synth, use*)

van Leusen, A.M. *et al.*, *Tet. Lett.*, 1972, 2367, (*synth, ir, pmr*)

Org. Synth., 1977, **57**, 102, (*synth*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 377; 1988, **13**, 313; **10**, 409; **8**, 493; **12**, 511; **11**, 539, (*use*)

van Leusen, A.M., *Lect. Heterocycl. Chem.*, 1980, **5**, 5111, (*rev*)

van Leusen, A.M. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1985, **104**, 50

Lamberth, C., *J. Prakt. Chem.*, 1998, **340**, 483-485, (*rev*)