



>>Entry Name: Methyl phenyl sulfide, 8Cl

ENTRY UNDER REVIEW

Synonym(s): (Methylthio)benzene, 9Cl. Thioanisole. Methylmercaptobenzene

CAS Registry Number: 100-68-5

PhSMe

Molecular Formula: C₇H₈S

Molecular Weight: 124.206

Accurate Mass: 124.03467

Percentage Composition: C 67.69%; H 6.49%; S 25.82%

Use/Importance: Used in *ortho*-formylation of anilines. A polymeric form can be used for Corey-Kim oxidn. of primary and secondary alcohols

Physical Description: Oil

Melting Point: Fp -15°

Boiling Point: Bp 188° (194-196°). Bp₆ 58-60°

Density: d₄²⁵ 1.053

Refractive Index: n_D²⁰ 1.5865

Hazard & Toxicity: Irritant. LD₅₀ (rat, orl) 891 mg/kg

Aldrich: T2800-2

Fluka: 88470

Sigma: T2765

>>Derivative: S-Oxide

>>Derivative: S,S-Dioxide

Synonym(s): Methyl phenyl sulfone. (Methylsulfonyl)benzene, 9Cl

CAS Registry Number: 3112-85-4

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

Physical Description: Plates (H₂O)

Melting Point: Mp 88°

Fluka: 68742

Rare Chemicals Library: S41550-2

References:

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