



>>Entry Name: 2,5-Dimethylthiophene, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 638-02-8

Type of Compound Code(s): WE9999

Structure by analogy with 2,3-Dimethylthiophene, FWX55-D

Molecular Formula: C₆H₈S

Molecular Weight: 112.195

Accurate Mass: 112.03467

Percentage Composition: C 64.23%; H 7.19%; S 28.58%

Use/Importance: Odorant used in food flavouring

Melting Point: Fp -62.6°

Boiling Point: Bp 136.8°

Solubility: Insol. H₂O; sol. Et₂O, EtOH, C₆H₆

Density: d²⁰ 0.985

Refractive Index: n_D²⁰ 1.5129

Aldrich: D18860-3

Fluka: 41670

>>Derivative: Dioxide

CAS Registry Number: 50590-79-9

Molecular Formula: C₆H₈O₂S

Molecular Weight: 144.194

Accurate Mass: 144.0245

Percentage Composition: C 49.98%; H 5.59%; O 22.19%; S 22.24%

Physical Description: Cryst.

Melting Point: Mp 88°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 44C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 592C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1467D, (*ir*)

Adv. Chem. Ser., 1955, **15**, 190, (*props*)

Jean, G.N. *et al.*, *J.O.C.*, 1955, **20**, 1363, (*synth*)

Jeffery, G.H. *et al.*, *J.C.S.*, 1961, 570

Lanum, W.J. *et al.*, *J. Chem. Eng. Data*, 1969, **14**, 93, (*ms, ir, uv, Raman*)

Nishimura, H. *et al.*, *J.O.C.*, 1975, **40**, 1567, (*synth, ms, ir, pmr*)

Rozen, S. *et al.*, *Chem. Comm.*, 1994, 1959, (*dioxide*)