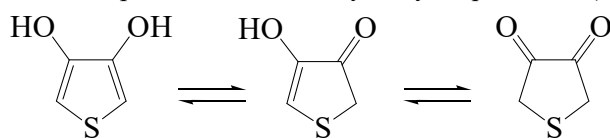




>>Entry Name: 3,4-Thiophenediol

Synonym(s): 4-Hydroxy-3(2*H*)-thiophenone, 8Cl. Dihydro-3,4-thiophenedione. 3,4-Dihydroxythiophene. 3,4(2*H*,5*H*)-Thiophenedione



CAS Registry Number: 33688-12-9

Molecular Formula: C₄H₄O₂S

Molecular Weight: 116.14

Accurate Mass: 115.9932

Percentage Composition: C 41.37%; H 3.47%; O 27.55%; S 27.61%

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 90-91° (89-91°)

Other Data: Dec. on exposure to heat, light and moisture

>>Variant: Diol-form

Molecular Formula: C₄H₄O₂S

Molecular Weight: 116.14

Accurate Mass: 115.9932

Percentage Composition: C 41.37%; H 3.47%; O 27.55%; S 27.61%

>>Derivative: Dibenzoyl

Molecular Formula: C₁₈H₁₂O₄S

Molecular Weight: 324.356

Accurate Mass: 324.04563

Percentage Composition: C 66.65%; H 3.73%; O 19.73%; S 9.89%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 109.5-110°

>>Derivative: Di-Me ether

Synonym(s): 3,4-Dimethoxythiophene, 8Cl

CAS Registry Number: 51792-34-8

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 23-24°

Boiling Point: Bp₂₀ 105°. Bp_{0.05} 55-57°

Density: d₄²⁵ 1.21

Refractive Index: n_D²⁰ 1.5409

>>Derivative: Di-*tert*-butyl ether

Synonym(s): 3,4-Di-*tert*-butoxythiophene

CAS Registry Number: 33688-11-8

Molecular Formula: C₁₂H₂₀O₂S

Molecular Weight: 228.355

Accurate Mass: 228.1184

Percentage Composition: C 63.12%; H 8.83%; O 14.01%; S 14.04%

Boiling Point: Bp_{0.2} 70-71°

Refractive Index: n_D²⁰ 1.4875

References:

- Fager, E.W., *J.A.C.S.*, 1945, **67**, 2217-2218, (*synth, dibenzoyl*)
Gogte, V.N. *et al.*, *Tetrahedron*, 1967, **23**, 2437-2441, (*synth*)
Martensen, J.Z. *et al.*, *Tetrahedron*, 1971, **27**, 3839-3851, (*synth, ir, uv, pmr, di-tert-butyl ether*)
Keegstra, M.A. *et al.*, *Tetrahedron*, 1992, **48**, 3633-3652, (*di-Me ether*)
Merz, A. *et al.*, *J. Prakt. Chem.*, 1996, **338**, 672-674, (*di-Me ether, synth, ir, uv, pmr, cmr, ms*)
Goldoni, F. *et al.*, *Synth. Commun.*, 1998, **28**, 2237-2244, (*di-Me ether, synth, ir, pmr, cmr*)