>>**Entry Name: 1,3-Benzenedithiol,** 9CI
Synonym(s): Dithioresorcinol. *m*-Dimercaptobenzene. 1,3-Disulfydrylbenzene

CAS Registry Number: 626-04-0

Molecular Formula: $C_6H_6S_2$
Molecular Weight: 142.245
Accurate Mass: 141.99109
Percentage Composition: C 50.66%; H 4.25%; S 45.09%
Physical Description: Leaflets
Melting Point: Mp 27° (25°)
Boiling Point: Bp 245°. $Bp_{0.2}$ 62°

Aldrich: 26909-3
Fluka: 38491

>>**Derivative:** 1,3,5-Trinitrobenzene complex

Physical Description: Yellow cryst.
Melting Point: Mp 76-77°

>>**Derivative:** Di-Ac

CAS Registry Number: 24197-87-3
Molecular Formula: $C_{10}H_{10}O_2S_2$
Molecular Weight: 226.32
Accurate Mass: 226.01222
Percentage Composition: C 53.07%; H 4.45%; O 14.14%; S 28.34%
Other Data: No Mp reported

>>**Derivative:** *S*-Me
Synonym(s): 3-(Methylthio)benzenethiol, 9CI

CAS Registry Number: 65144-65-2
Molecular Formula: $C_7H_8S_2$
Molecular Weight: 156.272
Accurate Mass: 156.00674
Percentage Composition: C 53.80%; H 5.16%; S 41.04%
Boiling Point: $Bp_{1.5}$ 98-101°

>>**Derivative:** *S*,*S*'-Di-Me
Synonym(s): 1,3-Bis(methylthio)benzene, 9CI

CAS Registry Number: 2388-69-4
Molecular Formula: $C_8H_{10}S_2$
Molecular Weight: 170.299
Accurate Mass: 170.02239
Percentage Composition: C 56.42%; H 5.92%; S 37.66%
Boiling Point: $Bp_{0.2}$ 90-92°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 421C, *(nmr)*
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1177C, *(ir)*
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1094B, *(ir)*
Marziano, N. *et al.*, *Ann. Chim. (Rome)*, 1962, **52**, 121; 143, *(ir, uv)*
Vögtle, F. *et al.*, *Chem. Ber.*, 1973, **106**, 719, *(synth, pmr)*
Kurth, H.J. *et al.*, *Chem. Ber.*, 1973, **106**, 2419, *(synth)*
Del Buttero, P. *et al.*, *J.O.C.*, 1983, **48**, 3114, *(synth, deriv)*