



>>Entry Name: Benzenesulfonylthioic acid, 9CI

Synonym(s): Thiobenzenesulfonic acid, 8CI. Benzenethiolsulfonic acid

CAS Registry Number: 13431-03-3

Related CAS Registry Numbers(s): 1887-29-2

PhSO<sub>2</sub>SH

Molecular Formula: C<sub>6</sub>H<sub>6</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 174.244

Accurate Mass: 173.98092

Percentage Composition: C 41.36%; H 3.47%; O 18.36%; S 36.81%

General Statement: Free acid unknown

Other Data: Aq. soln. dec. to PhSO<sub>2</sub>H + S

>>Derivative: Me ester

Synonym(s): S-Methyl benzenethiosulfonate

CAS Registry Number: 1125-25-3

Molecular Formula: C<sub>7</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 188.271

Accurate Mass: 187.99657

Percentage Composition: C 44.66%; H 4.28%; O 17.00%; S 34.06%

Physical Description: Liq.

Boiling Point: Bp<sub>1</sub> 123°

>>Derivative: Et ester

CAS Registry Number: 1127-31-7

Molecular Formula: C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 202.298

Accurate Mass: 202.01222

Percentage Composition: C 47.50%; H 4.98%; O 15.82%; S 31.70%

Physical Description: Oil

Boiling Point: Bp<sub>0.15</sub> 104-106°. Bp<sub>0.1</sub> 90-91°

>>Derivative: Benzyl ester

CAS Registry Number: 16601-01-7

Molecular Formula: C<sub>13</sub>H<sub>12</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 264.369

Accurate Mass: 264.02787

Percentage Composition: C 59.06%; H 4.57%; O 12.10%; S 24.26%

Physical Description: Cryst. (CCl<sub>4</sub>/hexane)

Melting Point: Mp 43°

>>Derivative: Ph ester

Synonym(s): S-Phenyl benzenethiosulfonate

CAS Registry Number: 1212-08-4

Molecular Formula: C<sub>12</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>

Molecular Weight: 250.342

Accurate Mass: 250.01222

Percentage Composition: C 57.57%; H 4.03%; O 12.78%; S 25.62%

Use/Importance: Sulfonylating agent

Physical Description: Cryst. (MeOH)

Melting Point: Mp 44-45° (36-37°)

Aldrich: 39026-7

Fluka: 12801

#### References:

Abe, Y. *et al.*, *Chem. Lett.*, 1972, 441, (*synth*)

Meier, H. *et al.*, *Synthesis*, 1972, 267, (*synth*)

Trost, B.M. *et al.*, *J.A.C.S.*, 1977, **99**, 4405, (*synth*)

Bhattacharya, A.K. *et al.*, *J.O.C.*, 1978, **43**, 2728, (*synth*, *pmr*, *cmr*)

Kim, Y.H. *et al.*, *Tet. Lett.*, 1978, 1211; 2305, (*synth*)

Takata, T. *et al.*, *Tet. Lett.*, 1978, 4303, (*pmr*)

Fieser and Fieser's *Reagents for Organic Synthesis*, Wiley, 1980, **8**, 391

Oae, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 2484, (*synth*, *ir*, *pmr*)