>>**Entry Name: 2-Mercaptobenzoic acid**
**Synonym(s): Thiosalicylic acid‡**


**CAS Registry Number:** 147-93-3
**Related CAS Registry Numbers(s):** 74010-85-8

**Molecular Formula:** $C_7H_6O_2S$
**Molecular Weight:** 154.189
**Accurate Mass:** 154.00885
**Percentage Composition:** C 54.53%; H 3.92%; O 20.75%; S 20.80%
**Use/Importance:** Used in manuf. of thioindigo dyes. Analgesic. Used as 2% Py soln. for extraction-photometric detn. of Co (ε 16500), Pd ($\lambda_{max}$ 370 nm, ε 17000, $CHCl_3$)
**Physical Description:** Yellow leaflets or needles (EtOH aq.)
**Melting Point:** Mp 165.5°
**Solubility:** Sol. Py
**pKa Value:** p$K_{a1}$ 3.54; p$K_{a2}$ 8.6 (25°) p$K_a$ 5.02 (48.9% EtOH)
**Calculated Log P Data:** Log P 2.44 (calc)
**Other Data:** Used as Na salt (Reocyl)
**Hazard & Toxicity:** $LD_{50}$ (mus, ipr) 50 mg/kg

**Aldrich:** T3320-0
**Fluka:** 89040
**Sigma:** T7500

>>**Derivative:** Me ester

**CAS Registry Number:** 4892-02-8
**Molecular Formula:** $C_8H_8O_2S$
**Molecular Weight:** 168.216
**Accurate Mass:** 168.0245
**Percentage Composition:** C 57.12%; H 4.79%; O 19.02%; S 19.06%
**Physical Description:** Oil
**Boiling Point:** $Bp_{728}$ 262-263°. $Bp_{11}$ 123°
**Other Data:** Steam-volatile

**Aldrich:** 35775-8

>>**Derivative:** Ph ester
**Synonym(s):** Phenyl 2-mercaptobenzoate. Thiosalol

**CAS Registry Number:** 15570-18-0
**Molecular Formula:** $C_{13}H_{10}O_2S$
**Molecular Weight:** 230.287
**Accurate Mass:** 230.04015
**Percentage Composition:** C 67.80%; H 4.38%; O 13.90%; S 13.92%
**Physical Description:** Needles (MeOH)
**Melting Point:** Mp 91°

>>**Derivative:** Amide
**Synonym(s):** Thiosalicylamide. 2-Mercaptobenzamide

**CAS Registry Number:** 5697-20-1

**Molecular Formula:** $C_7H_7NOS$
**Molecular Weight:** 153.204
**Accurate Mass:** 153.024834
**Percentage Composition:** C 54.88%; H 4.61%; N 9.14%; O 10.44%; S 20.93%
**Use/Importance:** Used as a 1% soln. in 20% aq. EtOH for extraction-photometric and gravimetric detn. of Au, Ir, Os, Pt, Rh, Ru, Ta ($\lambda_{max}$ 460 nm, $CHCl_3$)
**Physical Description:** Cryst. (hot $H_2O$)
**Melting Point:** Mp 121°

>>**Derivative:** Ac
**Synonym(s):** Thioaspirin