



>>Entry Name: Chloromethanesulfonic acid

CAS Registry Number: 40104-07-2

ClCH₂SO₃H

Molecular Formula: CH₃ClO₃S

Molecular Weight: 130.552

Accurate Mass: 129.949142

Percentage Composition: C 9.20%; H 2.32%; Cl 27.16%; O 36.77%; S 24.56%

>>Derivative: Na salt

CAS Registry Number: 10352-63-3

Physical Description: Cryst. (MeOH)

Melting Point: Mp 261-262.5°

>>Derivative: Benzylthiuronium salt

Physical Description: Cryst. (H₂O)

Melting Point: Mp 97-98°

>>Derivative: Chloride

Synonym(s): Chloromethanesulfonyl chloride

CAS Registry Number: 3518-65-8

Molecular Formula: CH₂Cl₂O₂S

Molecular Weight: 148.997

Accurate Mass: 147.915254

Percentage Composition: C 8.06%; H 1.35%; Cl 47.59%; O 21.48%; S 21.52%

Physical Description: Liq.

Boiling Point: Bp₂₅ 80-81°

Hazard & Toxicity: Lachrymator, severe skin and eye irritant. LD₅₀ (rat, orl) 372 mg/kg

Rare Chemicals Library: S61687-7

>>Derivative: Bromide

Synonym(s): Chloromethanesulfonyl bromide

Molecular Formula: CH₂BrClO₂S

Molecular Weight: 193.448

Accurate Mass: 191.884738

Percentage Composition: C 6.21%; H 1.04%; Br 41.31%; Cl 18.33%; O 16.54%; S 16.58%

Physical Description: Oil

Boiling Point: Bp_{0.6} 50-54°

References:

Smith, T.L. *et al.*, *J.A.C.S.*, 1953, **75**, 3566, (*synth*)

Org. Synth., Coll. Vol., 5, 1973, 231, (*deriv, synth*)

Silhanek, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1977, **42**, 524, (*synth, pmr*)

Block, E. *et al.*, *J.A.C.S.*, 1986, **108**, 4568, (*deriv, synth, ir, pmr, use*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CHY000