



>>Entry Name: Benzylsulfonic acid

Synonym(s): Phenylmethanesulfonic acid, 9CI. α -Toluenesulfonic acid, 8CI

CAS Registry Number: 100-87-8

PhCH₂SO₃H

Molecular Formula: C₇H₈O₃S

Molecular Weight: 172.204

Accurate Mass: 172.019415

Percentage Composition: C 48.82%; H 4.68%; O 27.87%; S 18.62%

Physical Description: Hygroscopic cryst.

>>Derivative: Me ester

CAS Registry Number: 5877-96-3

Molecular Formula: C₈H₁₀O₃S

Molecular Weight: 186.231

Accurate Mass: 186.035065

Percentage Composition: C 51.60%; H 5.41%; O 25.77%; S 17.22%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 61-62°

>>Derivative: Et ester

CAS Registry Number: 42454-54-6

Molecular Formula: C₉H₁₂O₃S

Molecular Weight: 200.258

Accurate Mass: 200.050715

Percentage Composition: C 53.98%; H 6.04%; O 23.97%; S 16.01%

Physical Description: Oil

>>Derivative: Ph ester

CAS Registry Number: 10271-81-5

Molecular Formula: C₁₃H₁₂O₃S

Molecular Weight: 248.302

Accurate Mass: 248.050715

Percentage Composition: C 62.88%; H 4.87%; O 19.33%; S 12.91%

Melting Point: Mp 87°

>>Derivative: Fluoride

CAS Registry Number: 329-98-6

Molecular Formula: C₇H₇FO₂S

Molecular Weight: 174.195

Accurate Mass: 174.015078

Percentage Composition: C 48.27%; H 4.05%; F 10.91%; O 18.37%; S 18.41%

Use/Importance: Reagent used for prepn. of benzylsulfonate esters used in synth.

Hazard & Toxicity: LD₅₀ (mus, orl) 200 mg/kg

Aldrich: 23479-6

Fluka: 78830

Sigma: P2567

>>Derivative: Chloride

CAS Registry Number: 1939-99-7

Molecular Formula: C₇H₇ClO₂S

Molecular Weight: 190.65

Accurate Mass: 189.985527

Percentage Composition: C 44.10%; H 3.70%; Cl 18.60%; O 16.78%; S 16.82%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 93°

Aldrich: 15971-9

Fluka: 78826