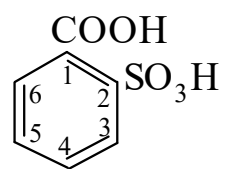




>>Entry Name: 2-Sulfobenzoic acid, 9CI

Synonym(s): Benzoic acid *o*-sulfonic acid. 2-Carboxybenzenesulfonic acid



CAS Registry Number: 632-25-7

Related CAS Registry Numbers(s): 14945-31-4 62574-72-5 123333-68-6

Molecular Formula: C₇H₆O₅S

Molecular Weight: 202.187

Accurate Mass: 201.993595

Percentage Composition: C 41.58%; H 2.99%; O 39.57%; S 15.86%

Physical Description: Cryst. + 3H₂O (H₂O)

Melting Point: Mp 68-69°. Mp 134° (anhyd.)

Other Data: Heat → anhydride

>>Derivative: Mono-NH₄ salt

CAS Registry Number: 6939-89-5

Melting Point: Mp 265-266°

>>Derivative: Bis(benzylthiuronium) salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 205-206°

>>Derivative: C-Me ester, *S*-chloride

Synonym(s): Methyl 2-(chlorosulfonyl)benzoate, 9CI. 2-(Methoxycarbonyl)benzenesulfonyl chloride

CAS Registry Number: 26638-43-7

Molecular Formula: C₈H₇ClO₄S

Molecular Weight: 234.66

Accurate Mass: 233.975357

Percentage Composition: C 40.95%; H 3.01%; Cl 15.11%; O 27.27%; S 13.66%

Physical Description: Cryst.

Melting Point: Mp 64-65°

>>Derivative: C-Me ester, *S*-amide

Synonym(s): Methyl 2-(aminosulfonyl)benzoate, 9CI. 2-(Methoxycarbonyl)benzenesulfonamide

CAS Registry Number: 57683-71-3

Molecular Formula: C₈H₉NO₄S

Molecular Weight: 215.229

Accurate Mass: 215.025229

Percentage Composition: C 44.64%; H 4.21%; N 6.51%; O 29.73%; S 14.90%

Physical Description: Cryst.

Melting Point: Mp 125-126°

Aldrich: 24523-2

>>Derivative: C-Et ester, *S*-chloride

Synonym(s): Ethyl 2-(chlorosulfonyl)benzoate, 9CI. 2-(Ethoxycarbonyl)benzenesulfonyl chloride

Molecular Formula: C₉H₉ClO₄S

Molecular Weight: 248.686

Accurate Mass: 247.991007

Percentage Composition: C 43.47%; H 3.65%; Cl 14.26%; O 25.73%; S 12.89%

Physical Description: Oil