



>>Entry Name: (3-Nitrophenyl)methanesulfonic acid

Synonym(s): 3-Nitrobenzenemethanesulfonic acid, 9Cl. *m*-Nitrotoluene- α -sulfonic acid. 3-Nitrobenzylsulfonic acid

Molecular Formula: C₇H₇NO₅S

Molecular Weight: 217.202

Accurate Mass: 217.004494

Percentage Composition: C 38.71%; H 3.25%; N 6.45%; O 36.83%; S 14.76%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 74°

>>Derivative: Me ester

Molecular Formula: C₈H₉NO₅S

Molecular Weight: 231.229

Accurate Mass: 231.020144

Percentage Composition: C 41.56%; H 3.92%; N 6.06%; O 34.60%; S 13.87%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 99-100°

>>Derivative: Chloride

CAS Registry Number: 58032-84-1

Molecular Formula: C₇H₆ClNO₄S

Molecular Weight: 235.647

Accurate Mass: 234.970606

Percentage Composition: C 35.68%; H 2.57%; Cl 15.04%; N 5.94%; O 27.16%; S 13.61%

Physical Description: Rhombic cryst. (C₆H₆)

>>Derivative: Amide

Molecular Formula: C₇H₈N₂O₄S

Molecular Weight: 216.217

Accurate Mass: 216.020478

Percentage Composition: C 38.89%; H 3.73%; N 12.96%; O 29.60%; S 14.83%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 159 dec.°

References:

Purgotti, A. *et al.*, *Gazz. Chim. Ital.*, 1900, **30**, 246

Clutterbuck, P.W. *et al.*, *J.C.S.*, 1923, **123**, 2507

Ingold, C.K. *et al.*, *J.C.S.*, 1927, 813