



>>Entry Name: 4-Sulfobutanoic acid, 9Cl

CAS Registry Number: 62605-67-8

Extra CAS Registry Numbers(s): 29508-18-7

HOOCCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>SO<sub>3</sub>H

Molecular Formula: C<sub>4</sub>H<sub>8</sub>O<sub>5</sub>S

Molecular Weight: 168.17

Accurate Mass: 168.009245

Percentage Composition: C 28.57%; H 4.79%; O 47.57%; S 19.07%

Physical Description: Cryst. + 0.5H<sub>2</sub>O (H<sub>2</sub>O)

Melting Point: Mp 93-93.5° (hemihydrate)

>>Derivative: S-Benzylisothiouronium salt

Melting Point: Mp 160.6-161.4°

>>Derivative: Di-Me ester

Molecular Formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>S

Molecular Weight: 196.224

Accurate Mass: 196.040545

Percentage Composition: C 36.73%; H 6.16%; O 40.77%; S 16.34%

Boiling Point: Bp 150-153°

>>Derivative: S-Chloride, C-Me ester

Synonym(s): Methyl 4-(chlorosulfonyl)butanoate, 9Cl. 3-(Methoxycarbonyl)propanesulfonyl chloride

CAS Registry Number: 81926-28-5

Molecular Formula: C<sub>5</sub>H<sub>9</sub>ClO<sub>4</sub>S

Molecular Weight: 200.642

Accurate Mass: 199.991007

Percentage Composition: C 29.93%; H 4.52%; Cl 17.67%; O 31.90%; S 15.98%

Physical Description: Liq.

Boiling Point: Bp<sub>0.65</sub> 98-99°

>>Derivative: Dichloride

Synonym(s): 4-(Chlorosulfonyl)butanoyl chloride. 3-(Chlorocarbonyl)propanesulfonyl chloride

CAS Registry Number: 62635-89-6

Molecular Formula: C<sub>4</sub>H<sub>6</sub>Cl<sub>2</sub>O<sub>3</sub>S

Molecular Weight: 205.061

Accurate Mass: 203.941469

Percentage Composition: C 23.43%; H 2.95%; Cl 34.58%; O 23.41%; S 15.64%

Physical Description: Oil

Boiling Point: Bp<sub>0.01</sub> 100-120° (bath)

>>Derivative: S-Amide

Synonym(s): 4-(Aminosulfonyl)butanoic acid. 3-Carboxypropanesulfonamide

CAS Registry Number: 175476-52-5

Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO<sub>4</sub>S

Molecular Weight: 167.185

Accurate Mass: 167.025229

Percentage Composition: C 28.74%; H 5.43%; N 8.38%; O 38.28%; S 19.18%

Physical Description: Solid

Melting Point: Mp 93-95°

>>Derivative: S-Amide, C-Me ester

Synonym(s): Methyl 4-(aminosulfonyl)butanoate, 9Cl. Methyl 4-sulfamoylbutanoate. 3-(Methoxycarbonyl)propanesulfonamide

CAS Registry Number: 175476-51-4

Molecular Formula: C<sub>5</sub>H<sub>11</sub>NO<sub>4</sub>S

Molecular Weight: 181.212

Accurate Mass: 181.040879

Percentage Composition: C 33.14%; H 6.12%; N 7.73%; O 35.32%; S 17.70%

Physical Description: Solid

Melting Point: Mp 49-50°