>>**Entry Name: 4-Sulfobutanoic acid,** 9CI

CAS Registry Number: 62605-67-8
Extra CAS Registry Numbers(s): 29508-18-7
$HOOCCH_2CH_2CH_2SO_3H$

Molecular Formula: $C_4H_8O_5S$
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. + $0.5H_2O$ (H_2O)
Melting Point: Mp 93-93.5° (hemihydrate)

>>**Derivative:** *S*-Benzylisothiouronium salt

Melting Point: Mp 160.6-161.4°

>>**Derivative:** Di-Me ester

Molecular Formula: $C_6H_{12}O_5S$
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, 9CI. 3-(Methoxycarbonyl)propanesulfonyl chloride

CAS Registry Number: 81926-28-5
Molecular Formula: $C_5H_9ClO_4S$
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: $Bp_{0.65}$ 98-99°

>>**Derivative:** Dichloride
Synonym(s): 4-(Chlorosulfonyl)butanoyl chloride. 3-(Chlorocarbonyl)propanesulfonyl chloride

CAS Registry Number: 62635-89-6
Molecular Formula: $C_4H_6Cl_2O_3S$
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: $Bp_{0.01}$ 100-120° (bath)

>>**Derivative:** *S*-Amide
Synonym(s): 4-(Aminosulfonyl)butanoic acid. 3-Carboxypropanesulfonamide

CAS Registry Number: 175476-52-5
Molecular Formula: $C_4H_9NO_4S$
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, 9CI. Methyl 4-sulfamoylbutanoate. 3-(Methoxycarbonyl)propanesulfonamide

CAS Registry Number: 175476-51-4
Molecular Formula: $C_5H_{11}NO_4S$
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°