



>>Entry Name: 1,3-Propanedisulfonic acid, 9CI

**CAS Registry Number:** 21668-77-9

HO3SCH2CH2CH2SO3H

**Molecular Formula:** C<sub>3</sub>H<sub>8</sub>O<sub>6</sub>S<sub>2</sub>

**Molecular Weight:** 204.225

**Accurate Mass:** 203.97623

**Percentage Composition:** C 17.64%; H 3.95%; O 47.01%; S 31.40%

**Physical Description:** Needles

**Boiling Point:** Bp<sub>1.4</sub> 157°

**Solubility:** Sol. H<sub>2</sub>O, EtOH

**Other Data:** Dec. without melting at 92°

**Sigma:** P8454

>>Derivative: Dichloride

**CAS Registry Number:** 20686-91-3

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

**Molecular Weight:** 241.115

**Accurate Mass:** 239.908454

**Percentage Composition:** C 14.94%; H 2.51%; Cl 29.41%; O 26.54%; S 26.60%

**Melting Point:** Mp 45°

>>Derivative: Anhydride

**Molecular Formula:** C<sub>6</sub>H<sub>14</sub>O<sub>11</sub>S<sub>2</sub>

**Molecular Weight:** 326.302

**Accurate Mass:** 325.997755

**Percentage Composition:** C 22.09%; H 4.32%; O 53.94%; S 19.65%

**Physical Description:** Solid by subl.

**Melting Point:** Mp 193-196 dec.°

>>Derivative: Diamide

**CAS Registry Number:** 13427-51-5

**Molecular Formula:** C<sub>3</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>

**Molecular Weight:** 202.255

**Accurate Mass:** 202.008198

**Percentage Composition:** C 17.82%; H 4.98%; N 13.85%; O 31.64%; S 31.71%

**Physical Description:** Cryst. (H<sub>2</sub>O or EtOH)

**Melting Point:** Mp 169°

#### References:

Zuffanti, S. *et al.*, *J.A.C.S.*, 1941, **63**, 2999, (*synth*)

McElvain, S.M. *et al.*, *J.A.C.S.*, 1946, **67**, 1580, (*synth*)

Geiseler, G. *et al.*, *Chem. Ber.*, 1958, **91**, 1512, (*synth*)