



>>Entry Name: **2,4-Dimethylbenzenesulfonic acid**, 9Cl  
Synonym(s): 2,4-Xylenesulfonic acid, 8Cl. *m*-Xylene-4-sulfonic acid

CAS Registry Number: 88-61-9  
Related CAS Registry Numbers(s): 827-21-4  
Extra CAS Registry Numbers(s): 1300-72-7 25321-41-9  
Structure by analogy with 2,3-Dimethylbenzenesulfonic acid, [DSX21-S](#)

Molecular Formula: C<sub>8</sub>H<sub>10</sub>O<sub>3</sub>S  
Molecular Weight: 186.231  
Accurate Mass: 186.035065  
Percentage Composition: C 51.60%; H 5.41%; O 25.77%; S 17.22%  
Physical Description: Plates or prisms + 2H<sub>2</sub>O (H<sub>2</sub>O)  
Melting Point: Mp 61-62°

Rare Chemicals Library: S55977-6

>>Derivative: Fluoride

CAS Registry Number: 445-15-8  
Molecular Formula: C<sub>8</sub>H<sub>9</sub>FO<sub>2</sub>S  
Molecular Weight: 188.222  
Accurate Mass: 188.030728  
Percentage Composition: C 51.05%; H 4.82%; F 10.09%; O 17.00%; S 17.04%  
Boiling Point: Bp 246°. Bp<sub>15</sub> 149-150°

>>Derivative: Chloride

CAS Registry Number: 609-60-9  
Molecular Formula: C<sub>8</sub>H<sub>9</sub>ClO<sub>2</sub>S  
Molecular Weight: 204.677  
Accurate Mass: 204.001177  
Percentage Composition: C 46.95%; H 4.43%; Cl 17.32%; O 15.63%; S 15.67%  
Physical Description: Cryst.  
Melting Point: Mp 34°

>>Derivative: Amide

CAS Registry Number: 7467-12-1  
Molecular Formula: C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub>S  
Molecular Weight: 185.246  
Accurate Mass: 185.051049  
Percentage Composition: C 51.87%; H 5.98%; N 7.56%; O 17.27%; S 17.31%  
Physical Description: Needles (H<sub>2</sub>O)  
Melting Point: Mp 138-139°

>>Derivative: Anhydride

CAS Registry Number: 58811-91-9  
Molecular Formula: C<sub>16</sub>H<sub>18</sub>O<sub>5</sub>S<sub>2</sub>  
Molecular Weight: 354.447  
Accurate Mass: 354.059565  
Percentage Composition: C 54.22%; H 5.12%; O 22.57%; S 18.09%  
Melting Point: Mp 139°  
Other Data: Dec. on standing

#### References:

Patterson, T.S. *et al.*, *J.C.S.*, 1924, **125**, 2488, (*synth*)  
Pollak, J. *et al.*, *Monatsh. Chem.*, 1928, **50**, 237, (*synth*)  
Huntress, E.H. *et al.*, *J.A.C.S.*, 1941, **63**, 3446, (*synth*)  
*Czech. Pat.*, 1976, 165 237; *CA*, **86**, 139621, (*synth*)  
El Homsy, A. *et al.*, *J. Chromatogr.*, 1978, **151**, 413, (*glc*)  
Roemmele, R.C. *et al.*, *J.O.C.*, 1988, **53**, 2367, (*chloride, synth, pmr, ir*)  
Lefebvre, J. *et al.*, *Acta Cryst. C*, 1992, **48**, 612, (*cryst struct*)  
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, XJJ000