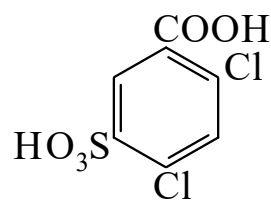




>>Entry Name: 2,4-Dichloro-5-sulfobenzoic acid



Molecular Formula: C₇H₄Cl₂O₅S

Molecular Weight: 271.077

Accurate Mass: 269.915649

Percentage Composition: C 31.02%; H 1.49%; Cl 26.16%; O 29.51%; S 11.83%

>>Derivative: 5-Amide

CAS Registry Number: 2736-23-4

Molecular Formula: C₇H₅Cl₂NO₄S

Molecular Weight: 270.092

Accurate Mass: 268.931633

Percentage Composition: C 31.13%; H 1.87%; Cl 26.25%; N 5.19%; O 23.69%; S 11.87%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 235-236° (230-232°)

Aldrich: 14739-7

>>Derivative: 5-Amide, Me ester

CAS Registry Number: 5046-15-1

Molecular Formula: C₈H₇Cl₂NO₄S

Molecular Weight: 284.119

Accurate Mass: 282.947283

Percentage Composition: C 33.82%; H 2.48%; Cl 24.96%; N 4.93%; O 22.52%; S 11.29%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 202°

>>Derivative: 5-Amide, Et ester

CAS Registry Number: 4793-25-3

Molecular Formula: C₉H₉Cl₂NO₄S

Molecular Weight: 298.146

Accurate Mass: 296.962933

Percentage Composition: C 36.26%; H 3.04%; Cl 23.78%; N 4.70%; O 21.47%; S 10.76%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 116°

>>Derivative: 5-Amide, 1-chloride

CAS Registry Number: 3740-16-7

Molecular Formula: C₇H₄Cl₃NO₃S

Molecular Weight: 288.538

Accurate Mass: 286.897745

Percentage Composition: C 29.14%; H 1.40%; Cl 36.86%; N 4.85%; O 16.63%; S 11.11%

Physical Description: Cryst. (petrol)

Melting Point: Mp 175-176°

>>Derivative: 5-Amide, hydrazide

CAS Registry Number: 18648-15-2

Molecular Formula: C₇H₇Cl₂N₃O₃S

Molecular Weight: 284.122

Accurate Mass: 282.958516

Percentage Composition: C 29.59%; H 2.48%; Cl 24.96%; N 14.79%; O 16.89%; S 11.29%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 248-249°