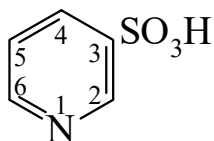




>>Entry Name: 3-Pyridinesulfonic acid, 9Cl, 8Cl



CAS Registry Number: 636-73-7

Molecular Formula: C₅H₅NO₃S

Molecular Weight: 159.165

Accurate Mass: 158.999014

Percentage Composition: C 37.73%; H 3.17%; N 8.80%; O 30.16%; S 20.15%

Use/Importance: Niacin antimetabolite

Physical Description: Needles, plates, cryst. (EtOH aq.)

Melting Point: Mp 365-370° (338-339°, 357°)

Solubility: V. sol. H₂O, spar. sol. EtOH, insol. Et₂O

pKa Value: pK_a 2.9 (2325°,23)

Aldrich: P6480-4

Fluka: 82820

Sigma: P6767

>>Derivative: NH₄ salt

Physical Description: Cryst.

Melting Point: Mp 243°

>>Derivative: Chloride

CAS Registry Number: 16133-25-8

Molecular Formula: C₅H₄ClNO₂S

Molecular Weight: 177.611

Accurate Mass: 176.965126

Percentage Composition: C 33.81%; H 2.27%; Cl 19.96%; N 7.89%; O 18.02%; S 18.05%

Boiling Point: Bp₂₀ 134-136°

>>Derivative: Chloride; hydrochloride

CAS Registry Number: 42899-76-3

Molecular Formula: C₅H₅Cl₂NO₂S

Molecular Weight: 214.071

Percentage Composition: C 28.05%; H 2.35%; Cl 33.12%; N 6.54%; O 14.95%; S 14.98%

Melting Point: Mp 141-144 dec.°

>>Derivative: Amide

CAS Registry Number: 2922-45-4

Molecular Formula: C₅H₆N₂O₂S

Molecular Weight: 158.181

Accurate Mass: 158.014998

Percentage Composition: C 37.97%; H 3.82%; N 17.71%; O 20.23%; S 20.27%

Melting Point: Mp 110-111°

>>Derivative: Diethylamide

Molecular Formula: C₉H₁₄N₂O₂S

Molecular Weight: 214.288

Accurate Mass: 214.077598

Percentage Composition: C 50.45%; H 6.58%; N 13.07%; O 14.93%; S 14.96%

Melting Point: Mp 49-50°