



>>Entry Name: 4-Pyridinesulfonic acid, 9Cl

CAS Registry Number: 5402-20-0

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%

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

Melting Point: Mp 134-135°. Mp 317-318 dec.°

>>Derivative: Amide

CAS Registry Number: 65938-88-7

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%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 172-173°

>>Derivative: N-Oxide

CAS Registry Number: 5402-22-2

Molecular Formula: C₅H₅NO₄S

Molecular Weight: 175.165

Accurate Mass: 174.993929

Percentage Composition: C 34.28%; H 2.88%; N 8.00%; O 36.54%; S 18.31%

Physical Description: Cryst./EtOH

Melting Point: Mp 326-328°

>>Derivative: N-Fluoro, zwitterion

Synonym(s): N-Fluoropyridinium-4-sulfonate

Molecular Formula: C₅H₄FNO₃S

Molecular Weight: 177.156

Accurate Mass: 176.989592

Percentage Composition: C 33.90%; H 2.28%; F 10.72%; N 7.91%; O 27.09%; S 18.10%

Use/Importance: Fluorinating reagent

Physical Description: Cryst.

Melting Point: Mp 230-260 dec.°

References:

den Hertog, H.J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 963, (*synth, uv*)

Org. Synth., 1963, **43**, 97, (*synth*)

Umemoto, T. *et al.*, *J.O.C.*, 1995, **60**, 6563, (*N-fluoro, synth, pmr, F-19 nmr, ir*)