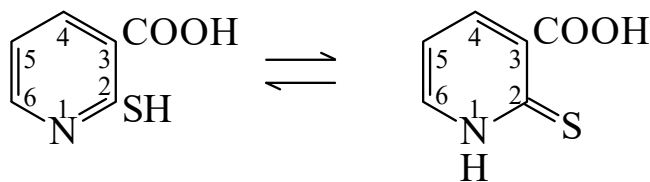




>>Entry Name: 2-Mercapto-3-pyridinecarboxylic acid, 9Cl

Synonym(s): 1,2-Dihydro-2-thioxo-3-pyridinecarboxylic acid, 9Cl. 2(1*H*)-Pyridinethione-3-carboxylic acid. 2-Mercaptonicotinic acid, 8Cl



CAS Registry Number: 38521-46-9

Molecular Formula: C₆H₅NO₂S

Molecular Weight: 155.177

Accurate Mass: 155.004099

Percentage Composition: C 46.44%; H 3.25%; N 9.03%; O 20.62%; S 20.66%

Physical Description: Cryst. (H₂O), yellow needles (EtOH aq.)

Melting Point: Mp 270° (260-261° dec.)

Aldrich: 41970-2

Fluka: 63763

>>Derivative: Hydrazide

Molecular Formula: C₆H₇N₃OS

Molecular Weight: 169.207

Accurate Mass: 169.030982

Percentage Composition: C 42.59%; H 4.17%; N 24.83%; O 9.46%; S 18.95%

Physical Description: Cryst. (DMF/EtOH)

Melting Point: Mp 330°

>>Derivative: Amide

Molecular Formula: C₆H₆N₂OS

Molecular Weight: 154.192

Accurate Mass: 154.020083

Percentage Composition: C 46.74%; H 3.92%; N 18.17%; O 10.38%; S 20.80%

Melting Point: Mp 260-262° (245-247°)

Other Data: Not obt. completely pure of elemental S.

>>Derivative: Nitrile

Synonym(s): 3-Cyano-2-pyridinethiol. 2-Mercapto-3-cyanopyridine

Molecular Formula: C₆H₄N₂S

Molecular Weight: 136.177

Accurate Mass: 136.009518

Percentage Composition: C 52.92%; H 2.96%; N 20.57%; S 23.55%

Physical Description: Yellow needles (EtOAc)

Melting Point: Mp 217-220°

>>Variant: Thiol-form

Molecular Formula: C₆H₅NO₂S

Molecular Weight: 155.177

Accurate Mass: 155.004099

Percentage Composition: C 46.44%; H 3.25%; N 9.03%; O 20.62%; S 20.66%

>>Derivative: S-Me

CAS Registry Number: 74470-23-8

Molecular Formula: C₇H₇NO₂S

Molecular Weight: 169.204

Accurate Mass: 169.019749

Percentage Composition: C 49.69%; H 4.17%; N 8.28%; O 18.91%; S 18.95%

Melting Point: Mp 215-217°

Aldrich: 25108-9

References: