



>>Entry Name: 4-Isothiocyanatophenol, 9CI
Synonym(s): *p*-Hydroxyphenyl isothiocyanate, 8CI

CAS Registry Number: 2131-60-4

Molecular Formula: C₇H₅NOS
Molecular Weight: 151.189
Accurate Mass: 151.009184
Percentage Composition: C 55.61%; H 3.33%; N 9.26%; O 10.58%; S 21.21%
Use/Importance: Parent compd. and derivatives show pesticidal (including anthelmintic) props.
Physical Description: Pale yellow needles
Melting Point: Mp 43-44°
Boiling Point: Bp₁₁ 175-185°. Bp_{0.3} 119-122°
Solubility: Insol. Et₂O, sol. EtOH, C₆H₆

>>Derivative: *O*-Ac

CAS Registry Number: 4061-59-0
Molecular Formula: C₉H₇NO₂S
Molecular Weight: 193.226
Accurate Mass: 193.019749
Percentage Composition: C 55.94%; H 3.65%; N 7.25%; O 16.56%; S 16.60%
Physical Description: Needles (H₂O)
Melting Point: Mp 38° (34°)

>>Derivative: *O*-Butanoyl

Molecular Formula: C₁₁H₁₁NO₂S
Molecular Weight: 221.279
Accurate Mass: 221.051049
Percentage Composition: C 59.71%; H 5.01%; N 6.33%; O 14.46%; S 14.49%
Melting Point: Mp 23°

>>Derivative: *O*-Benzoyl

CAS Registry Number: 3529-88-2
Molecular Formula: C₁₄H₉NO₂S
Molecular Weight: 255.297
Accurate Mass: 255.035399
Percentage Composition: C 65.87%; H 3.55%; N 5.49%; O 12.53%; S 12.56%
Melting Point: Mp 66°

>>Derivative: Me ether

Synonym(s): 1-Isothiocyanato-4-methoxybenzene, 9CI

CAS Registry Number: 2284-20-0
Molecular Formula: C₈H₇NOS
Molecular Weight: 165.215
Accurate Mass: 165.024834
Percentage Composition: C 58.16%; H 4.27%; N 8.48%; O 9.68%; S 19.41%
Physical Description: Cryst. (Et₂O)
Melting Point: Mp 28-30°
Boiling Point: Bp₈ 142°
Density: d 1.2
Refractive Index: n_D²⁰ 1.6470
Aldrich: 24718-9
Fluka: 65220
Other: Oakwood 1278

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-4-isothiocyanatobenzene