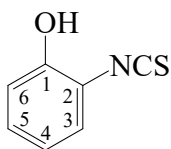




>>Entry Name: **2-Isothiocyanatophenol**, 9CI

Synonym(s): *o*-Hydroxyphenyl isothiocyanate



CAS Registry Number: 86695-08-1

Molecular Formula: C<sub>7</sub>H<sub>5</sub>NOS

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: Derivs. show pesticidal (including anthelmintic) activity

>>Derivative: Formyl

CAS Registry Number: 72695-33-1

Molecular Formula: C<sub>8</sub>H<sub>5</sub>NO<sub>2</sub>S

Molecular Weight: 179.199

Accurate Mass: 179.004099

Percentage Composition: C 53.62%; H 2.81%; N 7.82%; O 17.86%; S 17.89%

Physical Description: Needles (EtOAc)

Melting Point: Mp 155.5-157°

>>Derivative: Ac

CAS Registry Number: 72695-34-2

Molecular Formula: C<sub>9</sub>H<sub>7</sub>NO<sub>2</sub>S

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%

Boiling Point: Bp<sub>0.05</sub> 103-105°

>>Derivative: Me ether

Synonym(s): 1-Isothiocyanato-2-methoxybenzene, 9CI

CAS Registry Number: 3288-04-8

Molecular Formula: C<sub>8</sub>H<sub>7</sub>NOS

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%

Boiling Point: Bp 264-266°. Bp<sub>18</sub> 149°. Bp<sub>13</sub> 138-139°

Density: d 1.2

Refractive Index: n<sub>D</sub><sup>20</sup> 1.6458

Aldrich: 25370-7

Other: Oakwood 1276

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-2-isothiocyanatobenzene

CAS Registry Number: 23163-84-0

Molecular Formula: C<sub>9</sub>H<sub>9</sub>NOS

Molecular Weight: 179.242

Accurate Mass: 179.040484

Percentage Composition: C 60.31%; H 5.06%; N 7.81%; O 8.93%; S 17.89%

Boiling Point: Bp<sub>10</sub> 133°

>>Derivative: Trifluoromethyl ether

Synonym(s): 1-Isothiocyanato-2-(trifluoromethoxy)benzene. 2-(Trifluoromethoxy)phenyl isothiocyanate

CAS Registry Number: 175205-33-1

Molecular Formula: C<sub>8</sub>H<sub>4</sub>F<sub>3</sub>NOS

Molecular Weight: 219.187

Accurate Mass: 218.996568

Percentage Composition: C 43.84%; H 1.84%; F 26.00%; N 6.39%; O 7.30%; S 14.63%

Boiling Point: Bp 215°

Other Data: Not well documented