



>>Entry Name: Thiocyanic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Sulfocyanic acid. Hydrogen thiocyanate

CAS Registry Number: 463-56-9

Related CAS Registry Numbers(s): 302-04-5 593-84-0

HSC≡N

Molecular Formula: CHNS

Molecular Weight: 59.092

Accurate Mass: 58.982969

Percentage Composition: C 20.33%; H 1.71%; N 23.70%; S 54.26%

Source/Synthesis: Present in Cruciferae e.g. *Brassica* spp. Synth. from KNCS + KHSO<sub>4</sub>

Use/Importance: Antibacterial agent

Physical Description: Polymerises at −90°, stable in dil. aq. soln.

Melting Point: Mp −110°

Solubility: Sol. H<sub>2</sub>O, EtOH, Et<sub>2</sub>O

pKa Value: pK<sub>a</sub> −1.85 (25°)

>>Derivative: NH<sub>4</sub> salt

>>Derivative: Me ester

Synonym(s): Methyl thiocyanate

CAS Registry Number: 556-64-9

Molecular Formula: C<sub>2</sub>H<sub>3</sub>NS

Molecular Weight: 73.118

Accurate Mass: 72.998619

Percentage Composition: C 32.85%; H 4.14%; N 19.16%; S 43.85%

Physical Description: Liq.

Melting Point: Fp −91°

Boiling Point: Bp<sub>756</sub> 130.5°

Density: d<sup>15</sup> 1.077

Refractive Index: n<sub>D</sub><sup>15</sup> 1.0765

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 60 mg/kg. LD<sub>50</sub> (mus, ipr) 23 mg/kg

Aldrich: 14658-7

>>Derivative: Et ester

Synonym(s): Ethyl thiocyanate, 9CI

CAS Registry Number: 542-90-5

Molecular Formula: C<sub>3</sub>H<sub>5</sub>NS

Molecular Weight: 87.145

Accurate Mass: 87.014269

Percentage Composition: C 41.35%; H 5.78%; N 16.07%; S 36.80%

Physical Description: Liq.

Boiling Point: Bp 146°

Solubility: Insol. H<sub>2</sub>O

Density: d<sup>16</sup> 1.02

Hazard & Toxicity: LD<sub>50</sub> (mus, ipr) 10 mg/kg

Aldrich: 30895-1

Fluka: 4880

Rare Chemicals Library: S60300-7