

D. MONOGRAPHS

Allyl Isothiocyanate

Volatile Oil of Mustard



C₄H₅NS

Mol. Wt. 99.16

2-propene isothiocyanate

[57-06-7]

Content Allyl Isothiocyanate contains not less than 97.0% of allyl isothiocyanate (C₄H₅NS).

Description Allyl Isothiocyanate is a transparent and colorless to light yellow liquid having a strong and irritating mustard-like odor.

Identification (1) Measure 3 ml of Allyl Isothiocyanate, add gradually 4 ml of sulfuric acid while cooling, and shake. A gas is evolved. The solution is transparent yellow, gradually becoming viscous, and the strong, irritating mustard-like odor disappears.

(2) To 2 ml of Allyl Isothiocyanate, add 3 ml of ethanol and 4 ml of ammonia TS, warm to about 50 °C, and allow to stand. The solution is transparent at first, but after about 3 hours, crystals appear.

Purity (1) Refractive index n_D^{20} : 1.528 - 1.531

(2) Specific gravity 1.018 - 1.023

(3) Phenols and thiocyanate compounds Measure 1.0 ml of Allyl Isothiocyanate, dissolve in 5 ml of ethanol, and add 1 drop of ferric chloride solution (1 : 10). Neither red nor blue color develops.

Assay Weigh accurately about 3 g of Allyl Isothiocyanate, and dissolve in ethanol to make exactly 100 ml. Measure exactly 5 ml of this solution, add 5 ml of ammonia TS, and add 50 ml of 0.1 mol/l silver nitrate, exactly measured. Equip with a reflux condenser, and heat for 1 hour in a water bath. Cool, add water to make exactly 100 ml, and filter through a dry filter paper. Discard about 10 ml of the initial filtrate, then measure exactly 50 ml of the subsequent filtrate, add 5 ml of nitric acid and 2 ml of ferric ammonium sulfate TS, and titrate the excess silver nitrate with 0.1 mol/l ammonium thiocyanate. Perform a blank test in the same manner.

1 ml of 0.1 mol/l silver nitrate = 4.958 mg of C₄H₅NS