

Chemical Information:

Name: Allyl isothiocyanate

Date of Analysis: 03 February 2010

CAS No.: 57-06-7

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_202249

Lot No.: 01308CE

NTP_CID No.: 472

MW: 99.15 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Thiocyanic acid, 2-propenyl ester (Allyl thiocyanate)	5.99	8.41
Allyl isothiocyanate	6.22	91.59

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

