

### Chemical Information:

Name: Benzyl isothiocyanate  
 CAS No.: 622-78-6  
 Tox21\_ID No.: Tox21\_201191  
 NTP\_CID No.: 4057  
 Supplier: Sigma-Aldrich  
 Lot No.: 19003TC  
 MW: 149.21 g/mol

Date of Analysis: 12 August 2009

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Benzyl isothiocyanate	14.40	100.00

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol
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	230°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Run Time	36.5 minutes
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

