

Chemical Information:

Name: Phenethyl isothiocyanate
CAS No.: 2257-09-2 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200100 Lot No.: 05311LH
NTP_CID No.: 4640 MW: 163.24 g/mol

Date of Analysis: 4 June 2014

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Phenethyl isothiocyanate	19.16	100.00

^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / Electron Impact
Solvent	Dichloromethane (~ 0.4 mg/mL)
Column	Zebron ZB-5MSi, 30 m x 0.32 mm ID, 0.5- μ m film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	30 – 375 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Split (100:1)
Run Time	59 minutes
Data Analysis Software	MSD ChemStation, ver D.03.00.SP1 and NIST Library ver 2.0, build 10/8/2008

