

Chemical Information:

Name: 3-Cyclohexene-1-methanol, .alpha.,.alpha.,4-trimethyl-
 CAS No.: 98-55-5 (alpha) Supplier: Alfa-Aesar
 586-81-2 (gamma)
 Tox21_ID No.: Tox21_200112 Lot No.: D18T039
 NTP_CID No.: 2596 MW: 154.25 g/mol

Date of Analysis: 4 June 2014

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	11.209	1.18
Unknown	11.278	1.84
3-Cyclohexene-1-methanol, .alpha.,.alpha.,4-trimethyl-, Alpha-	11.960	77.77
3-Cyclohexene-1-methanol, .alpha.,.alpha.,4-trimethyl-, Gamma-	12.148	19.21

^a Peaks comprising ≥ 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-μm 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 μL / Split (100:1)
Run Time	59 minutes
Data Analysis Software	MSD ChemStation, ver D.03.00.SP1 & F.01.01.2317 and NIST Library ver 2.0, build 10/8/2008 & 2.2 build 6/10/2014

