

Chemical Information:

Name: 3-Cyclohexene-1-methanol, .alpha., .alpha., 4-trimethyl-, acetate Date of Analysis: 07 August 2009
CAS No.: 80-26-2 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_202188 Lot No.: 04996EJ
NTP_CID No.: 2553 MW: 196.29 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	8.43	1.08
unknown	12.35	0.97
unknown	12.43	2.41
unknown	13.07	1.73
3-Cyclohexene-1-methanol, .alpha., .alpha., 4-trimethyl-, acetate	13.34	92.87

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol (~ 1 mg/mL)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m 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 μ L / Split (100:1)
Run Time	36.5 minutes
Data Analysis Software	Xcalibur, ver 1.2 and NIST Library ver 2.0f, build 10/08/2008

