

### Chemical Information:

Name: 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3E)-  
CAS No.: 79-77-6 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_201454 Lot No.: 08828BJ  
NTP\_CID No.: 2341 MW: 192.30 g/mol

Date of Analysis: 12 August 2009

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	14.35	0.73
3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3E)-	15.14	99.27

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  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- $\mu$ 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 $\mu$ L / Split (100:1)
Run Time	36.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

