

Chemical Information:

Name: 2-Butenal, 3-methyl-

Date of Analysis: 30 September 2009

CAS No.: 107-86-8

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_200149

Lot No.: 62496DJ

NTP_CID No.: 3834

MW: 84.12 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
2-Butenal, 3-methyl-	4.78	97.37
unknown	5.67	2.63

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
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	150°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

