

**Chemical Information:**

Name: Isosafrole (TGMX)  
 CAS No.: 120-58-1  
 Tox21\_ID No.: Tox21\_201783  
 NTP\_CID No.: 893

Supplier: Sigma-Aldrich  
 Lot No.: 00909AH  
 MW: 162.19 g/mol

Date of Analysis: 29 May 2009

**Purity and Identity Results:**

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Isosafrole (TGMX)	13.85	13.22
Isosafrole (TGMX)	14.37	86.57

<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	Methanol
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- $\mu$ m film thickness
Carrier Gas	Helium at 1.1 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	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (87:1)
Run Time	36.5 minutes
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

