

### Chemical Information:

Name: 1,4-Hexadiene  
CAS No.: 592-45-0  
Tox21\_ID No.: Tox21\_201155  
NTP CID No.: 2842

Supplier: Sigma-Aldrich  
Lot No.: 08206HY  
MW: 82.14 g/mol

Date of Analysis: 15 December 2009

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
1,4-Hexadiene	2.84	89.97
1,4-Hexadiene	2.90	7.47
unknown	9.83	1.10

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

Mixture of *cis* and *trans* isomers, per CoA; combined purity, 97.44%

**GC/MS Instrument Parameters:**

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Not applicable; analysis of neat chemical
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	10°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 µL / Split (480:1)
Data Analysis Software	Xcalibur, ver 1.2 and NIST Library ver 2.0f, build 10/08/2008

