

# Chemical Information:

Name: 2-Oxepanone  
CAS No.: 502-44-3  
Tox21\_ID No.: Tox21\_200445  
NTP\_CID No.: 2801

Supplier: Alfa Aesar  
Lot No.: 10140989  
MW: 114.14 g/mol

Date of Analysis: 21 August 2009

## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
2-Oxepanone	7.74	100.00

<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	70°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 (100:1)
Run Time	33.0 minutes
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

