

### Chemical Information:

Name: Propanoic acid, 2,2-dimethyl-, methyl ester Date of Analysis: 07 August 2009  
CAS No.: 598-98-1 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_200448 Lot No.: 13925LH  
NTP\_CID No.: 2846 MW: 116.16 g/mol

### Purity and Identity Results:

| Peak Identity                               | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|---|----------------------|------------------------------------|
| Propanoic acid, 2,2-dimethyl-, methyl ester | 3.20                 | 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 (~ 1 mg/mL)  |
| 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, ver 1.2 and NIST Library ver 2.0f, build 10/08/2008          |

