

### Chemical Information:

Name: Propanoic acid, 3-mercapto-, methyl ester  
CAS No.: 2935-90-2 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_200030 Lot No.: 06009ED  
NTP\_CID No.: 3030 MW: 120.17 g/mol

Date of Analysis: 10 September 2009

### Purity and Identity Results:

| Peak Identity                             | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|---|----------------------|------------------------------------|
| Propanoic acid, 3-mercapto-, methyl ester | 9.71                 | 96.25                              |
| Unknown                                   | 10.52                | 1.54                               |
| Unknown                                   | 20.58                | 1.33                               |

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

### GC/MS Instrument Parameters:

|                         |  |
|-------------------------|--|
| Instrument / Ionization | Gas Chromatograph with Mass Spectrometer / Electron Impact       |
| Solvent                 | Not applicable; analyzed 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, v 1.2 and NIST Library v 2.0f, build 10/08/2008        |

