

# Chemical Information:

Name: o-Nitrobenzyl chloride  
CAS No.: 612-23-7  
Tox21\_ID No.: Tox21\_200821  
NTP\_CID No.: 1116

Date of Analysis: 10 February 2009

Supplier: Sigma-Aldrich  
Lot No.: 11423CC  
MW: 171.58 g/mol

## Purity and Identity Results:

| Peak Identity          | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|------------------------|----------------------|------------------------------------|
| o-Nitrobenzyl chloride | 13.98                | 99.70                              |

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

## GC/MS Instrument Parameters:

|                         |  |
|-------------------------|--|
| Instrument / Ionization | Gas Chromatograph with Mass Spectrometer / Electron Impact       |
| Solvent                 | Dichloromethane  |
| 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            | 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 – 350 amu   |
| Injector Temperature    | 250°C  |
| Injection Volume / Mode | 1 μL / Split (10:1)  |
| Run Time                | 36.5 minutes   |
| Data Analysis Software  | Xcalibur, v 1.2 and NIST Library v 2.0, build 7/23/2008          |

