

### Chemical Information:

Name: Carbonochloridic acid, methyl ester  
CAS No.: 79-22-1 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_200841 Lot No.: 12730HD  
NTP\_CID No.: 2212 MW: 94.50 g/mol

Date of Analysis: 19 October 2010

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Carbonochloridic acid, methyl ester	2.81	97.53
Unknown	3.33	2.30

<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	Not applicable
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	10°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	200°C
Auxiliary Temperature	200°C
Scan Range	25 – 500 amu
Injector Temperature	150°C
Injection Volume / Mode	1 $\mu$ L / Split (350:1)
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

