

### Chemical Information:

Name: Phosphorochloridothioic acid, O,O-diethyl ester Date of Analysis: 10 September 2009  
CAS No.: 2524-04-1 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_200977 Lot No.: 03524MN  
NTP\_CID No.: 3013 MW: 188.61 g/mol

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Phosphorochloridothioic acid, O,O-diethyl ester	12.61	97.29
unknown	15.15	1.07

<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; analyzed neat chemical
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	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (480:1)
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

