

Chemical Information:

Name: o,o-Diethyl S-(((1,1-dimethylethyl)thio)methyl)phosphorodithioate Date of Analysis: 19 April 2007
CAS No.: 13071-79-9 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201634 Lot No.: 3036X
NTP_CID No.: 650 MW: 288.43 g/mol

Purity and Identity Results:

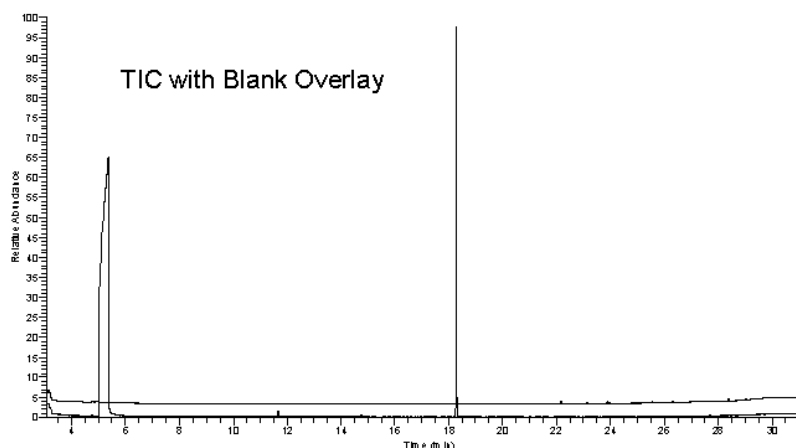
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.38	Not applicable
Unknown	11.67	1.21
o,o-Diethyl S-(((1,1-dimethylethyl)thio)methyl)phosphorodithioate	18.29	97.57

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with 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 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 350 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μL / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999

RT: 3.05-31.48 SM:3G



07-01953 #1833 RT: 18.29 AC: 1 NL: 33165
T: (p) + o EtS + 350.00 F48 ms (50.00-350.00)

