

Chemical Information:

Name: 2,6,6-Trimethyl-2-cyclohexene-1,4-dione Date of Analysis: 13 August 2015
CAS No.: 1125-21-9 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201193 Lot No.: S56137
NTP_CID No.: 5040 MW: 152.19 g/mol

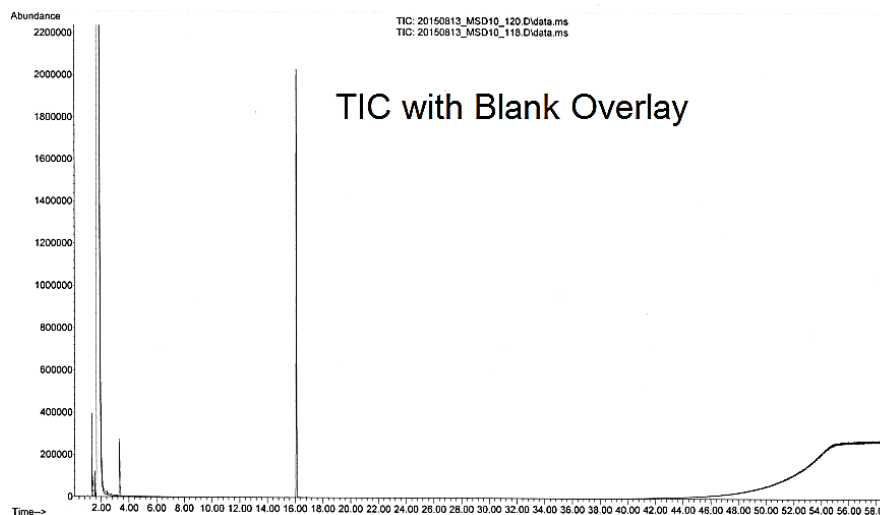
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
2,6,6-Trimethyl-2-cyclohexene-1,4-dione	16.10	99.69

^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

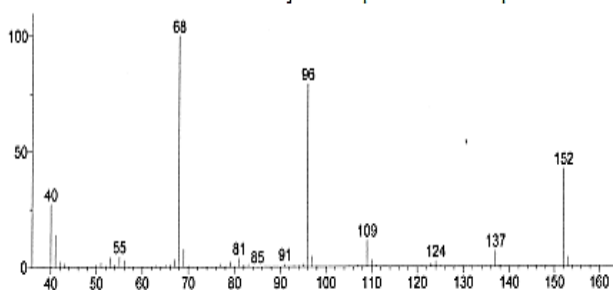
Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- μ m film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 550 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Splitless
Data Analysis Software	MSD ChemStation, ver D.03.00.611, NIST Library ver 2.0d, build Dec 2005



Unknown: Scan 2748 (16.105 min): 20150813_MSD10_120.D\data.ms
Compound in Library Factor = 405

Hit 1: 2,6,6-Trimethyl-2-cyclohexene-1,4-dione
C₉H₁₂O₂; MF: 958; RMF: 958; Prob 95.4%; CAS: 1125-21-9; Lib: replib; ID: 8360.

Major Component Mass Spectrum



NIST Reference Mass Spectrum

