

Chemical Information:

Name: 2,6,6-Trimethylcyclohexa-1,3-dienylmethanal
CAS No.: 116-26-7 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_202723 Lot No.: MKBC6469
NTP_CID No.: 6027 MW: 150.22 g/mol

Date of Analysis: 10 March 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	16.29	1.69	Unknown	16.96	0.83
Unknown	16.51	0.68	Unknown	17.01	0.73
CAS 116-26-7	16.64	93.76	Unknown	17.51	2.31

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1-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	40 – 640 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2 Build 2014

