

Chemical Information:

Name: 1,3-Propanedione, 1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)-
Date of Analysis: 21 March 2017
CAS No.: 70356-09-1 Supplier: TCI America
Tox21_ID No.: Tox21_202796 Lot No.: D75FA
NTP_CID No.: 5208 MW: 310.39 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	19.21	0.5
Unknown	19.81	1.09
Unknown	20.17	2.14
1,3-Propanedione, 1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)-	35.19	96.02

^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 – 550 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

x10⁶ + TIC Scan 20170321_MSD11_010.D

TIC with Blank Overlay

