

Chemical Information:

Name: Benzoic acid, 4-formyl-
CAS No.: 619-66-9 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_202478 Lot No.: 07026CJ
NTP_CID No.: 365 MW: 150.13 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	10.76	1.01	Benzoic acid, 4-formyl-	19.92	78.02
Unknown	13.77	1.07	Unknown	21.43	0.85
Unknown	14.61	2.08	Unknown	21.78	2.36
Unknown	17.52	1.61	Unknown	21.84	7.71
CAS 4122-56-9 ^b	19.03	5.02			

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

^b CAS 4122-56-9; Methyl 2-formylbenzoate

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- μ m 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 μ L / 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 20170310_MSD11_007.D

TIC with Blank Overlay

