

Chemical Information:

Name: Benzoic acid, 4-(bromomethyl)-, methyl ester
 CAS No.: 2417-72-3 Supplier: Sigma Aldrich
 Tox21_ID No.: Tox21_202815 Lot No.: MKBB5023V
 NTP_CID No.: 6126 MW: 229.07 g/mol

Date of Analysis: 21 March 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	16.86	0.59
Unknown	19.92	2.67
Unknown	20.33	1.25
Benzoic acid, 4-(bromomethyl)-, methyl ester	21.58	95.33

^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

