

### Chemical Information:

Name: Benzoic acid, 3-chloro-, methyl ester  
CAS No.: 2905-65-9 Supplier: Sigma Aldrich  
Tox21\_ID No.: Tox21\_201012 Lot No.: 03111AE  
NTP\_CID No.: 3028 MW: 170.59 g/mol

Date of Analysis: 11 August 2015

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Ethanol	1.50	Not applicable
Benzoic acid, 3-chloro-, methyl ester	19.55	100.00

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol (~ 400 µg/mL)
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1-µm film thickness
Carrier Gas	Helium at 2 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 750 amu
Injector Temperature	250°C
Injection Volume / Mode	1 µL / Split (10:1)
Run Time	59 minutes
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / Chemstation Enhanced Data Analysis F.01.01.2317 / NIST Library Version 2.2 Build 2014

