

### Chemical Information:

Name: Chloranil

Date of Analysis: 14 June 2016

CAS No.: 118-75-2

Supplier: Sigma-Aldrich

Tox21\_ID No.: Tox21\_201656

Lot No.: 09714EJ

NTP\_CID No.: 610

MW: 245.88 g/mol

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>	Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	4.61	0.99	Unknown	12.25	0.63
Unknown	8.52	0.51	Unknown	13.73	3.77
Unknown	9.55	0.52	Chloranil	31.86	92.37

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1-μm film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 550 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
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

