

### Chemical Information:

Name: 1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich  
 Date of Analysis: 15 April 2010  
 CAS No.: 68515-48-0 Supplier: Sigma-Aldrich  
 Tox21\_ID No.: Tox21\_202296 Lot No.: MKAA0039  
 NTP\_CID No.: 2408 MW: 418.61 g/mol

### Purity and Identity Results:

Peak Identity <sup>a</sup>	Retention Time (min)	Purity (% Total Area) <sup>b</sup>	Peak Identity <sup>a</sup>	Retention Time (min)	Purity (% Total Area) <sup>b</sup>
CAS # 20548-62-3	26.79	1.76	CAS # 20548-62-3	27.63	5.57
CAS # 20548-62-3	26.94	3.33	CAS # 20548-62-3	27.82	20.89
CAS # 20548-62-3	27.09	15.24	CAS # 20548-62-3	28.01	4.03
CAS # 20548-62-3	27.33	22.79	CAS # 20548-62-3	28.21	2.92
CAS # 20548-62-3	27.51	23.47			

<sup>a</sup> Per CoA, Diisononyl phthalate (mixture of C9 isomers), technical grade. Analysis yielded a number of unresolved components between 26.5 and 28.5 minutes. Based on mass spectra, components were identified as CAS # 20548-62-3 [phthalic acid, bis(7-methyloctyl) ester], indicating isomers of 1,2-benzenedicarboxylic acid with predominantly C9 branched alkyl esters. Total = 100.00% purity.

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

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane (~ 1 mg/mL)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- $\mu$ 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	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (100:1)
Data Analysis Software	Xcalibur ver 1.2, and NIST Library ver 2.0f, build 10/08/2008

