

Chemical Information:

Name: Pentaerythritol triacrylate Date of Analysis: 05 August 2010
CAS No.: 3524-68-3 Supplier: ABCR GmbH & Co.
Tox21_ID No.: Tox21_202024 Lot No.: 1136114
NTP_CID No.: 1170 MW: 298.29 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Related structure ^b	19.58	28.37	3524-68-3	22.16	55.16
Related structure ^b	20.84	12.55	unknown	25.71	3.91

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

^b CoA states 99.0% (total esters), without specifying components. Although not identified, based on similarities in spectra, component was included in purity.
Total = 96.08%.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- 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	230°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Split (100:1)
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

