

Chemical Information:

Name: Isophorone diisocyanate
 CAS No.: 4098-71-9 Supplier: Sigma Aldrich
 Tox21_ID No.: Tox21_201520 Lot No.: 03003PB
 NTP_CID No.: 883 MW: 222.28 g/mol

Date of Analysis: 07 October 2016

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Acetone	2.00	Not applicable
Isophorone diisocyanate	30.10	23.65
Isophorone diisocyanate	30.71	76.12

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone (~ 100 µg/mL)
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1-µm film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 475 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

x10⁷ + TIC Scan 20161007_MSD11_012.D

