

Chemical Information:

Name: 3-Chloropropionitrile

Date of Analysis: 08 May 2009

CAS No.: 542-76-7

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_202225

Lot No.: 05420PO

NTP_CID No.: 331

MW: 89.52 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
3-Chloropropionitrile	5.32	100.00

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone (~ 1 mg/mL)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.1 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 μL / Split (87.1:1)
Run Time	36.5 minutes
Data Analysis Software	MSD Chemstation ver D.03.00.SP1; NIST Library ver 2.0f, build 10/28/2008

