

Chemical Information:

Name: Heptanenitrile
CAS No.: 629-08-3
Tox21_ID No.: Tox21_200526
NTP_CID No.: 4989

Date of Analysis: 27 April 2015

Supplier: Sigma-Aldrich
Lot No.: 16509TU
MW: 111.18 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Ethanol	2.50	Not applicable
Heptanenitrile	14.23	100.00

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / Electron Impact
Solvent	Ethanol (~ 400 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 325°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 400 amu
Injector Temperature	250°C
Injection Volume / Mode	1 µL / Splitless
Run Time	60 minutes
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / Chemstation Enhanced Data Analysis F.01.01.2317 / NIST Library Version 2.2 Build 2014

