

# Chemical Information:

Name: 1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-  
CAS No.: 126-11-4 Supplier: Sigma Aldrich  
Tox21\_ID No.: Tox21\_200441 Lot No.: 09304DJ  
NTP\_CID No.: 2739 MW: 151.12 g/mol

Date of Analysis: 17 July 2015

## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Ethanol	1.50	Not applicable
1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-	22.89	99.79

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

## GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol (~ 400 $\mu\text{g/mL}$ )
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1- $\mu\text{m}$ film thickness
Carrier Gas	Helium at 2 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 600 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu\text{L}$ / Split (10:1)
Run Time	59 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

