

Chemical Information:

Name: Isobutyl nitrite
CAS No.: 542-56-3
Tox21_ID No.: Tox21_202411
NTP_CID No.: 877

Supplier: Sigma-Aldrich
Lot No.: 10806PH
MW: 103.12 g/mol

Date of Analysis: 25 March 2010

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	1.50	0.66
Isobutyl nitrite	2.97	78.29
1-Propanol, 2-methyl	3.64	8.92
Unknown	4.74	1.72
Unknown	6.49	0.96
Propanoic acid, 2-methyl-, 2-methylpropyl ester	9.18	6.20
Unknown	12.72	1.69

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Not applicable
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	10°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	200°C
Auxiliary Temperature	200°C
Scan Range	25 – 500 amu
Injector Temperature	200°C
Injection Volume / Mode	1 μ L / Split (420:1)
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

