

Chemical Information:

Name: 2-Methyl-2-butenenitrile
 CAS No.: 4403-61-6 Supplier: Sigma-Aldrich
 Tox21_ID No.: Tox21_200317 Lot No.: 208505/1
 NTP_CID No.: 260 MW: 81.12 g/mol

Date of Analysis: 25 October 2007

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.63	Not applicable
2-Methyl-3-butenenitrile	3.36	30.60
2-Methyl-2-butenenitrile	3.63	69.40

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
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	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 200 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μ L / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999

