

Chemical Information:

Name: Acetic acid, mercapto-, ethyl ester
CAS No.: 623-51-8 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_202860 Lot No.: 16004LO
NTP_CID No.: 6259 MW: 120.17 g/mol

Date of Analysis: 21 March 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	7.18	0.61
Acetic acid, mercapto-, ethyl ester	11.17	95.95
Unknown	22.38	3.45

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1- 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 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	40 – 550 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2 Build 2014

x10⁶ + TIC Scan 20170321_MSD11_010.D

