

Chemical Information:

Name: 4-Pentenoic acid, 3,3-dimethyl-, methyl ester Date of Analysis: 17 July 2015
CAS No.: 63721-05-1 Supplier: TCI America
Tox21_ID No.: Tox21_200468 Lot No.: GH01
NTP_CID No.: 3422 MW: 142.20 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Acetone	1.50	Not applicable
4-Pentenoic acid, 3,3-dimethyl-, methyl ester	8.79	100.00

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone (~ 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 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 µL / 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

