

Chemical Information:

| | | |
|---------------|---|-------------------------------|
| Name: | Propanoic acid, 2-methyl-, monoester with 2,2,4-trimethyl-1,3-pentanediol | Date of Analysis: 26 May 2015 |
| CAS No.: | 25265-77-4 | Supplier: Sigma-Aldrich |
| Tox21_ID No.: | Tox21_200148 | Lot No.: 39496TJ |
| NTP_CID No.: | 3252 | MW: 216.32 g/mol |

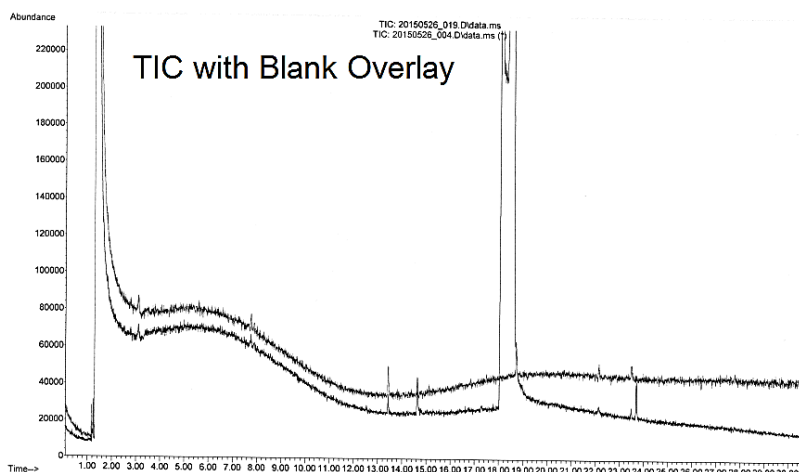
Purity and Identity Results:

| Peak Identity | Retention Time (min) | Purity (% Total Area) ^a |
|---|----------------------|------------------------------------|
| Propanoic acid, 2-methyl-, monoester with 2,2,4-trimethyl-1,3-pentanediol | 31.56 | 100.00 |

^a Peaks comprising ≥ 0.5% of total area.

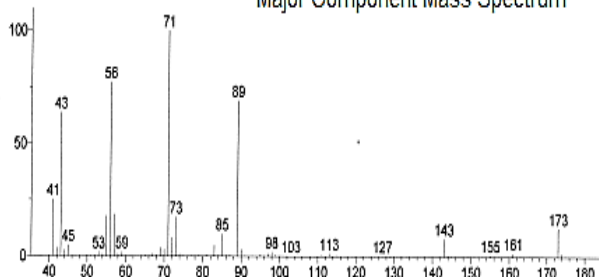
GC/MS Instrument Parameters:

| | |
|-------------------------|---|
| Instrument / Ionization | Gas Chromatograph with Mass Spectrometer / Electron Impact |
| Solvent | Ethanol |
| Column | Rxi-5Sil MS, 30 m x 0.25 mm ID, 0.50-μm film thickness |
| Carrier Gas | Helium at 1.5 mL/min |
| Oven Program | 50°C, hold 0 min; ramp @ 5°C/min to 300°C, hold 10 min |
| Source Temperature | 230°C |
| Auxiliary Temperature | 250°C |
| Scan Range | 40 – 600 amu |
| Injector Temperature | 250°C |
| Injection Volume / Mode | 1 μL / Splitless |
| Run Time | 58.0 minutes |
| Data Analysis Software | MSD ChemStation, ver D.03.00.611, NIST Library ver 2.0d, build Dec 2005 |



Unknown: Scan 2904 (18.563 min): 20150526_019.D\data.ms (-3037)
Compound in Library Factor = 388

Major Component Mass Spectrum



Hit 1: Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester
C₁₂H₂₄O₃; MF: 931; RMF: 931; Prob 92.5%; CAS: 77-68-3; Lib: mainlib; ID: 38750.

NIST Reference Mass Spectrum

