

Chemical Information:

Name: Hexanol, acetate, branched and linear
 CAS No.: 88230-35-7 Supplier: Sigma-Aldrich
 Tox21_ID No.: Tox21_200711 Lot No.: 04512TB
 NTP_CID No.: 2380 MW: 144.21 g/mol

Date of Analysis: 21 December 2009

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	7.39	0.66	Hexanol, acetate	8.25	15.46
Hexanol, acetate	7.94	1.79	Hexanol, acetate	8.32	26.06
Hexanol, acetate	8.09	13.62	Hexanol, acetate	8.85	37.08
Hexanol, acetate	8.16	3.22			

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	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 7 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Split (100:1)
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008

Abundance

