

Chemical Information:

Name: 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid,
7-oxabicyclo[4.1.0]hept-3-ylmethyl ester
CAS No.: 2386-87-0 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_202388 Lot No.: 02728AJ
NTP_CID No.: 3001 MW: 252.31 g/mol

Date of Analysis: 04 October 2016

Purity and Identity Results:

Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b	Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b
Acetone	2.00	Not applicable	2386-87-0	42.16	19.59
Unknown	38.01	3.14	Unknown	47.11	0.57
2386-87-0	41.70	56.60	Unknown	47.58	1.02
2386-87-0	42.12	15.85			

^a Three primary isomers identified; total = 92.04%.

^b Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone (~ 100 µg/mL)
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1-µm film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 475 amu
Injector Temperature	250°C
Injection Volume / Mode	1 µL / 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

