

Chemical Information:

Name: Isoxaben
CAS No.: 82558-50-7
Tox21_ID No.: Tox21_201574
NTP_CID No.: 2200

Date of Analysis: 13 October 2009

Supplier: Sigma-Aldrich
Lot No.: 8092X
MW: 332.39 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	5.73	3.54
Isoxaben	26.30	96.46

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol (~ 1 mg/mL)
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	250°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	Xcalibur, ver 1.2 and NIST Library ver 2.0f, build 10/08/2008

