

Chemical Information:

Name: Allyl thiourea
CAS No.: 109-57-9
Tox21_ID No.: Tox21_200898
NTP_CID No.: 474

Supplier: Sigma Aldrich
Lot No.: 06404CA
MW: 116.18 g/mol

Date of Analysis: 09 December 2009

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Allyl thiourea	10.4	100

^a Peaks comprising ≥ 0.5% of total area.

LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / ESI+
Solvent	Methanol
Column	Grace HP C18-AQ, 5 µm, 250 mm x 2.1 mm ID
Injection Volume	20 µL
Mobile Phase	95/5 (A) and 5/95 (B) Water/acetonitrile 2 mM ammonium formate, pH 3; acetonitrile (C)
Program / Flow Rate	100/0/0 A/B/C for 1 minute; 5/95/0 at 20 minutes, hold 2 minutes; 0/0/100 at 25 minutes, hold 3 minutes / 0.2 mL/minute
Cone / Capillary	25 V / 3.0 kV
Source Temperature	125°C
Desolve Temperature	325°C
Scan Range	100 – 1100 amu
Acquisition Software	MassLynx, v 4.0

