AR226-3270

Vapor Pressure Determination: [redacted]

DUPONT REPORT 12735

[redacted] **VAPOR PRESSURE**

Test Guideline(s)

Authors

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Study Completion Date

16 July 2002

Report Date

21 March 2003

Test Facility

DuPont Corporate Center for Analytical Sciences

Experimental Station 402/5321

Wilmington, DE 19880-0402

And

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Experimental Station 320

Wilmington, DE 19880-0320

Sponsor

Telomer Research Panel
c/o Rand Corporation

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1.0 SUMMARY

Test System:

[redacted] was used to determine its vapor pressure as a function of temperature.

Findings:

The vapor pressure at 23°C is approximately 3 Pa (0.022 Torr).

Conclusions:

The vapor pressure of [redacted] ranged from 3 Pa at 23°C to 101kPa at 201°C.

2.0 GENERAL STUDY INFORMATION

Study Objectives

The objective of this study was to determine the vapor pressure of [redacted] under defined conditions between 25°C and 200°C.

Test System Justification

The test system was determined by the sponsor.

Study Personnel

Management:	Marianne Marsi, Ph.D.
Study Director:	Mary A. Kaiser, Ph.D.
Principle Investigator:	Daryl P. Cobranchi, Ph.D.
Technical Personnel:	Barry W. Wolstenholme

Study Execution Dates

Study Initiation Date:	15-Jun-2001
Experimental Start Date:	15-Jun-2001
Experimental Completion Date:	28-June 2002
Study Completion Date:	12-July 2002

3.0 MATERIALS AND METHODS

3.1 Test Guidelines

The vapor pressure of a substance is defined as the saturation pressure above a solid or liquid substance. At thermodynamic equilibrium, the vapor pressure is only a function of temperature. The SI unit of pressure which should be used is the Pascal (Pa, Newton/m^2). Units which have been employed historically are 1 Torr (mm Hg) =1.33 x 10^2 Pa; 1 atmosphere = 1.013 x 10^5 Pa; 1 bar = 10^5 Pa. A modified OECD Guideline 104 (modified) was used for this measurement.

3.2.1 Chemical System

3.2.1.1 Test Substance

The test substance was obtained from Clariant Gmbh (Germany) and was shown to be [redacted] pure via gas chromatography. [redacted] impurities were detected. The major impurity [redacted] is tentatively identified as [redacted] based on the mass spectral fragmentation pattern.

Name: [redacted]

Synonym:

Active substance(s)

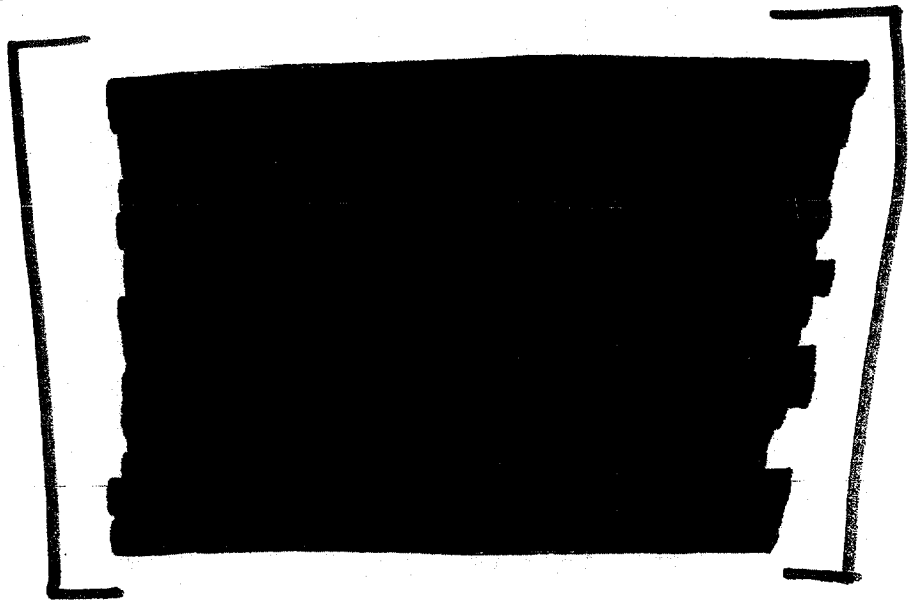
CAS Name:

CAS Number(s):

Company Sanitized. Does not contain TSCA CBI

Vapor Pressure Determination: [redacted]

Structure:



H Number	H-24691
Lot Number:	[redacted]
EMSE Sample Number:	
Concentration, nominal:	
Concentration, analyzed:	
Certificate of Analysis Date:	03-Apr. 2001
Date Received:	15-June -2001
Solubility at 25°C.:	~140 $\mu g\ L^{-1}$
Vapor pressure:	TBD via this report
Stability:	Stable at ambient room temperature
Appearance/Color:	White solid
Storage Conditions:	Room temperature; keep tightly closed

3.2.1.2 Test Vehicle

The test substance was the [redacted]

3.3 Test Conduct

Two techniques were used to obtain the vapor pressure. The first method was based on a dynamic measurement procedure by Scott[1] where the equilibrium temperature is measured at a controlled pressure. Approximately 30 grams of [redacted] was placed in a boiler. The pressure was held constant to 0.01% (0.01kPa) and measured to an accuracy of 0.01%. The apparatus consisted of a Mensor (San Marcos, TX) PCS400 pressure controller, a Paroscientific (Redmond, WA) 740 pressure transducer, and a Hart Scientific (American Fort UT) stack base unit for

temperature measurement. The temperature varied from 80 to 200°C. A diagram of the apparatus is given in Figure 2. Table 1 shows the individual data points.

The second procedure was based on the EPA OPPTS gas saturation method[2]. This second procedure is intended to confirm the linearity of the curve obtained at the higher temperatures from the Scott method. The [redacted] was placed directly in a glass thermostated tube. Gas-chromatographic grade helium [redacted] flowed over the powder. The flow was controlled by a flow controller on a Hewlett Packard (now Agilent, Little Falls, DE) model 5890 gas chromatograph. Due to the adsorptive properties of the [redacted] the vapor pressure was calculated from weight loss rather than from the weight of trapped material downstream. The vapor pressure at 21°C was 0.02 Torr. Figure 3 gives the vapor pressure curve obtained from both sets of measurements.

3.3 *Parameters Observed*

With the Scott apparatus, pressure and temperature are observed.

With the GC/MS apparatus, peak height and peak area are observed.

3.4 Result Analysis

With the GC/MS apparatus the peak height or area is compared to the same parameter of a standard carefuly prepared in methanol.

3.5 Validity Criteria of the Study

For GC/MS the peak areas of standards run before and after the test substance are compared. The results must agree within 5%.

4.0 RESULTS AND DISCUSSION

The vapor pressure of the [redacted] varied continuously from 3 Pa at 21°C to 101 kPa at 201°C. The results from the single point taken at 21°C were aligned with the results from the 11 points taken at elevated temperatures taken by the Scott method.

5.0 CONCLUSIONS

The vapor pressure of the [redacted] is 3 Pa at 21°C and 101 kPa at 201°C.

6.0 RETENTION OF RECORDS

Study documents and materials will be stored in the archives of the DuPont Experimental Station including but not limited to:

- study protocol;
- any protocol and/or report amendments or addenda or deviations;
- all raw data;
- one original signed copy of the final report;

- laboratory-specific or site-specific raw data such as personnel files, instrument, equipment, refrigerator, and/or freezer raw data.

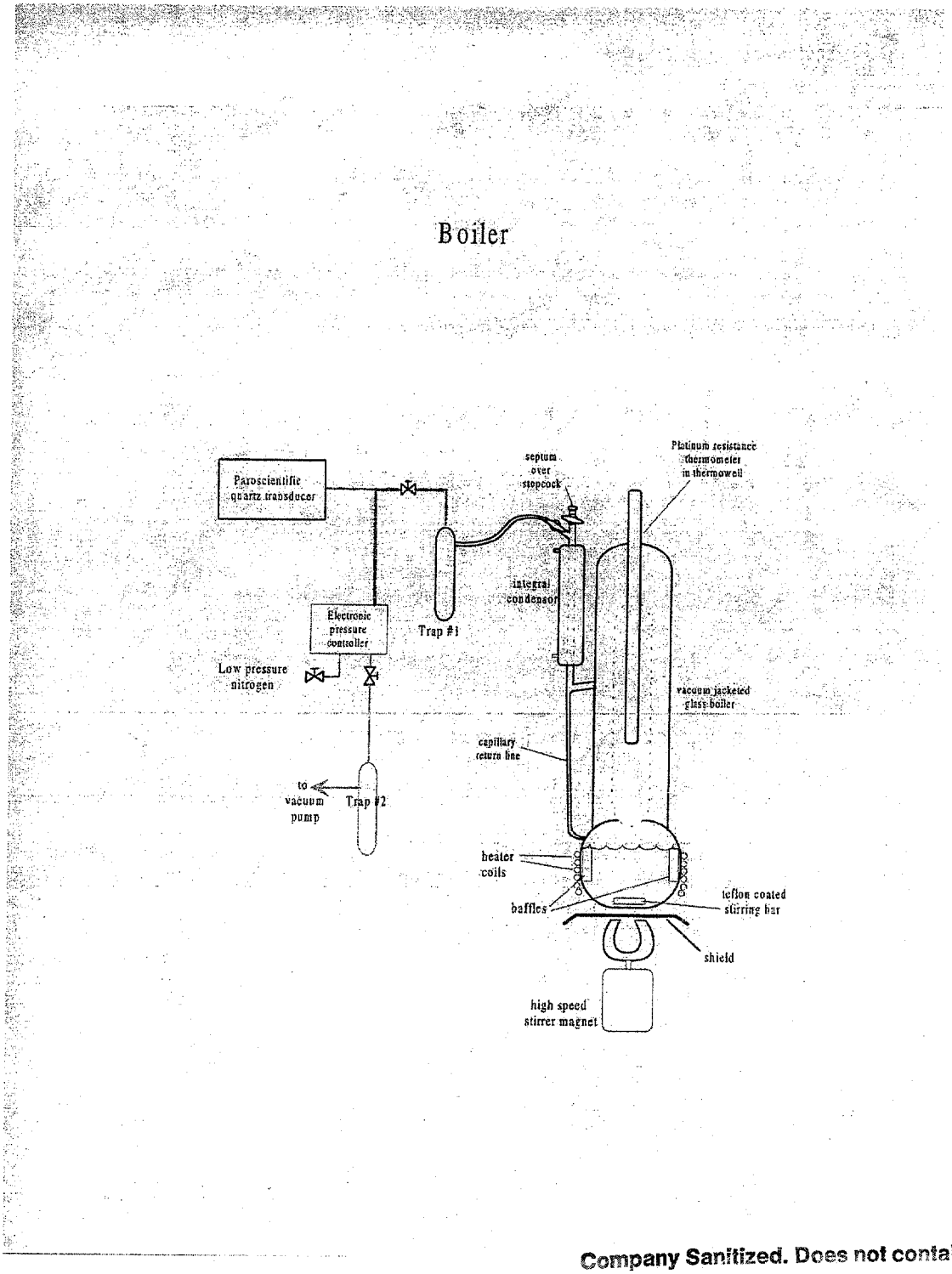
7.0 DISPOSAL OF TEST ITEM

After issuance of the final report, the remaining test substance will be stored at the DuPont Glasgow site until its expiration date and then destroyed by burning, unless other arrangements are made between the sponsor and the Test Facility.

8.0 REFERENCES

1. L. Scott, "Determination of Activity Coefficients by Accurate Measurement of Boiling Point Diagram", Fluid *Phase Equilibrium*, **26**,(1986), 149-163.
2. United States Environmental Protection Agency, Prevention, Pesticides and Toxic Substances (7101), OPPTS 830.7950, Vapor Pressure, August 1995, page 4, Gas Saturation Method.

Figure 1. Scott Method Apparatus



Company Sanitized. Does not contain TSCA CBI

Vapor Pressure Determination: [redacted]

Figure 2. Vapor Pressure: [redacted]

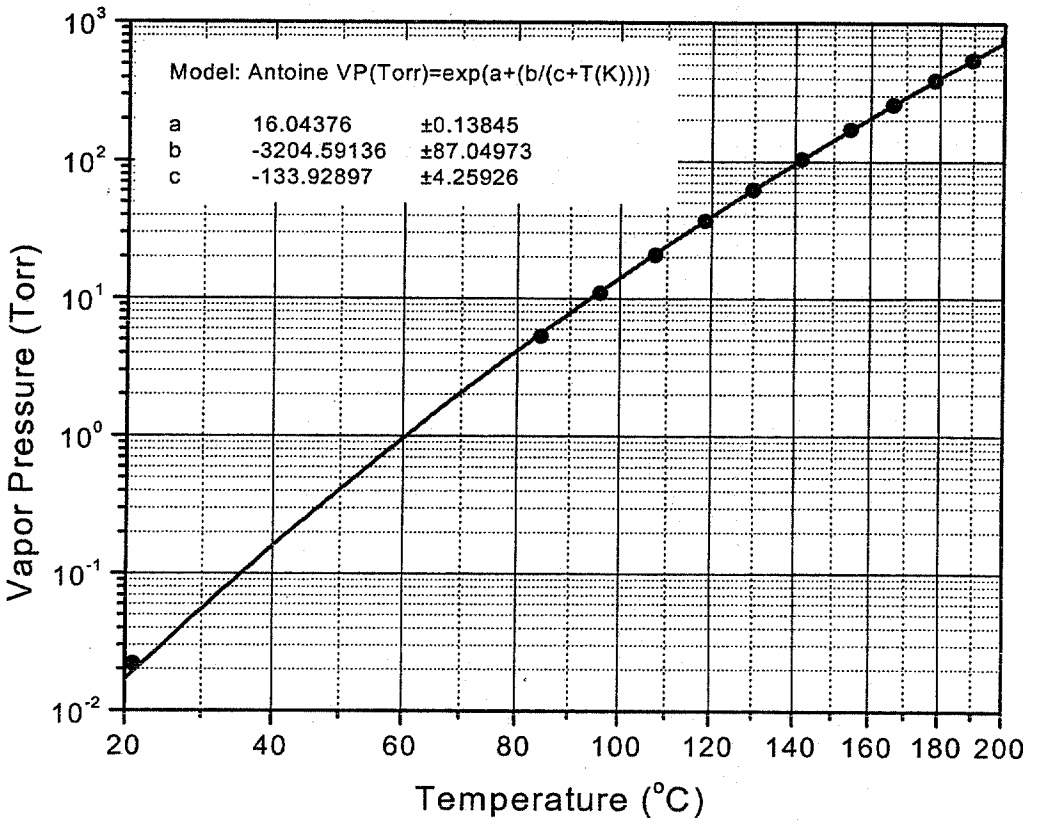


Table 1. Vapor Pressure Values

Temperature (C)	Vapor Pressure (Torr)	Vapor Pressure (Pa)	Method
21	0.022	3	Gas Saturation Method
84	5	708	Scott Method
96	11	1465	Scott Method
107	21	2774	Scott Method
119	37	4910	Scott Method
130	62	8284	Scott Method
142	103	13798	Scott Method
155	171	22752	Scott Method
166	258	34449	Scott Method
179	388	51667	Scott Method
190	543	72339	Scott Method
201	755	100607	Scott Method

Appendix A

Chemical Analysis Summary

[redacted]

Analysis Summary

The subject material was analyzed by gas-chromatography using a standard method to assess its composition. This analysis showed that the material comprised [redacted] of the subject material. The balance [redacted] was not [redacted] at a limit of quantitation of 0.02%. Further analysis by GC/MS suggests that the [redacted] is a single impurity, whose chemical structure is [redacted]

Finally, the subject material was evaluated by High Performance Liquid Chromatograpy - Tandem Mass Spectrometry (LC/MS/MS) for the presence of [redacted] at a detection limit of 0.1ppm. Neither material was observed to be present.

Based upon these analyses, we conclude that methods are in hand to determine and confirm the composition of H-24691 to be as follows:

Material	Wt. % (±0.3)
[redacted]	