

# **PROPICONAZOLE**

## **Dossier for Directive 98/8/EC Document IIIA**

### **Section 3 : Physical & Chemical Properties**

**From  
Tier I - Section 1 - Annex II  
of 91/414 dossier :  
Identity, chemistry data and  
general information**

Document IIIA – BPD 98/8	Section 3	PHYSICAL AND CHEMICAL PROPERTIES
91/414 Annex Point addressed	II 2	Physical and Chemical Properties of the Active Substance

### 3.1 Melting Point, Boiling Point, Relative density

#### 3.1.1 Freezing point

<b>General Information</b>	
<b>Title of the study:</b>	<b>Report on freezing temperature</b>
Project number:	PP-94 / 37P.MPR
Author:	A. Geoffroy
Syngenta file number (SAM):	64250 - 2441
Name and address of testing facility:	SYNGENTA., CH-4002 Basle, Switzerland
Date of report:	September 9, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.1
Test substance:	CGA 64250 pure
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The **freezing temperature** of the test substance (glass transition temperature of a liquid sample) was determined to be :

-23°C

Evaluation by Competent Authorities
1 December 2005. ██████████

#### 3.1.2 Boiling point

<b>General Information</b>	
<b>Title of the study:</b>	<b>Report on boiling point / boiling range</b>
Project number:	16313
Author:	R. Das
Syngenta file number (SAM):	64250 - 2290
Name and address of testing facility:	SYNGENTA Mönchwil AG, CH-4333 Mönchwil, Switzerland
Date of report:	November 8, 1993
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.2, OECD No. 103
Test substance:	CGA 64250 tech.
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

**Findings :**

The **boiling point** of the active substance was determined to be :

**>250°C (> 523 K) at 101.325 kPa**

**120°C (= 392.2 K) at 1.9 Pa.**

**Thermal decomposition begins around 355°C**

Evaluation by Competent Authorities	

**3.1.3 Relative density**

General Information	
<b>Title of the study:</b>	<b>Report on density</b>
Project number:	16314
Author:	R. Das
Syngenta file number (SAM):	64250 - 2289
Name and address of testing facility:	SYNGENTA Mönchwil AG, CH-4333 Mönchwil, Switzerland
Date of report:	November 8, 1993
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.3, OECD No. 109
Test substance:	CGA 64250 tech.
Batch identification:	
Purity of the test substance:	
Reliability indicator	1
Data Protection Claim	Yes

**Findings :**

The **density** of the test substance is

**1289 kg / m<sup>3</sup> (= 1.289 g / cm<sup>3</sup>) at 20°C**

Evaluation by Competent Authorities	

### 3.2 Vapour pressure, volatility

#### 3.2.1 Henry's law constant

<b>General Information</b>	
<b>Title of the study:</b>	<b>Report on vapour pressure curve</b>
Project number:	AG - 88 / 02 P
Author:	B.F. Rordorf / N. Burkhard
Syngenta file number (SAM):	64250 - 2087, 64250 - 2403
Name and address of testing facility:	SYNGENTA Ltd., CH-4002 Basle, Switzerland
Date of report:	June 15, 1988 / September 12, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	OECD No. 104
Test substance:	CGA 64250 pure
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The vapour pressure of propiconazole was determined to be

$$5.6 \cdot 10^{-5} \text{ Pa at } 25^{\circ}\text{C}$$

The Henry's Law Constant, H, is calculated from the following equation:

$$H = P_{VP} / S_W \quad [\text{Pa} \cdot \text{m}^3 / \text{mol}]$$

$P_{VP}$  = vapour pressure [Pa]

$S_W$  = water solubility [mol / m<sup>3</sup>]

The following data are used for the calculation of Henry's Law Constant for CGA 64250, propiconazole (mol. weight MW = 342.2 g/mol).

water solubility at 20°C : 100 g / m<sup>3</sup>

vapour pressure at 20°C : 2.7 · 10<sup>-5</sup> Pa

Based on these results **Henry's Law Constant** was estimated to be

$$9.2 \cdot 10^{-5} \text{ Pa} \cdot \text{m}^3 / \text{mol}$$

Evaluation by Competent Authorities	
20 April 2007.	

### 3.3 Appearance (physical state, colour and odour)

General Information	
<b>Title of the study:</b>	<b>Report on general physico-chemical properties</b>
Project number:	20751 (pure active ingredient) / 16311 (technical grade active ingredient)
Author:	R. Das
Syngenta file number (SAM):	64250- 2334 (pure a.i.) / 64250 - 2083 (technical grade a.i.)
Name and address of testing facility:	SYNGENTA Mönchwilten AG, CH-4333 Mönchwilten, Switzerland
Date of report:	March 22, 1994 (pure a.i.) / November 8, 1993 (technical grade a.i.)
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	visual and organoleptic test
Test substance:	CGA 64250
Batch identification:	
Purity of the test substance:	
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

Substance	Property		
	Colour	Aspect	Odour
Pure active ingredient	colourless	clear, viscous liquid	weak, slightly sweet
Technical grade active ingredient	yellowish	clear, viscous liquid	very slight mild odour

<b>Evaluation by Competent Authorities</b>
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1 December 2005. <span style="background-color: black; color: black;">[REDACTED]</span>
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### 3.4 Spectra (UV /VIS, IR, NMR, MS), Molecular extinction at relevant wavelengths

<b>General Information</b>	
<b>Title of the study:</b>	<b>Report on spectra</b>
Project number:	28042
Author:	W. Käser
Syngenta file number (SAM):	64250 - 2097
Name and address of testing facility:	SYNGENTA Mönchwil AG, CH-4333 Mönchwil, Switzerland
Date of report:	December 20, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	--
Test substance:	CGA 64250 pure
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

##### IR spectrum

- Operating procedures

Sample preparation : tel quel, between 2 NaCl plates  
 Instrument : Perkin Elmer 1420

- Peak list :

3000 - 3100 cm <sup>-1</sup>	(C - H) stretch	(aromatic)
2900 - 3000 cm <sup>-1</sup>	(C - H) stretch	(aliphatic)
1460 / 1500 / 1580 cm <sup>-1</sup>	(C - C) stretch	(aromatic)
1270 / 1130 / 1020 cm <sup>-1</sup>	(C - O -C) stretch	(asymmetric)

##### UV / VIS spectrum

- Operating procedures

Instrument : Hitachi U-3200      Concentration and solvent : 3.11 mg in 100 ml methanol  
 Quartz cell : 10 mm pathlength      Reference solvent : methanol

- List of characteristic bands

Wavelength [nm]	Molecular extinction coefficient [l · mol <sup>-1</sup> · cm <sup>-1</sup> ]
220.4	11666

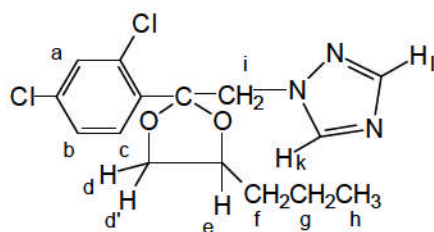
No absorption was observed between 340 nm and 750 nm

## H-NMR spectrum

### - Operating procedures

Operating temperature :	room temperature	Instrument :	Bruker ACF 300
Solvent :	DMSO	Nucleus :	<sup>1</sup> H (300 MHz)
		Internal standard :	TMS

### Structural formula



### - Table of chemical shifts

Chemical shift (ppm)	No. of Protons	Assignment	Multiplicity
0.85	3	h	two triplets (not resolved)
1.3	4	f, g	multiplet
3.25 / 3.35	1	d'	multiplets of diastereomeric forms
3.9 / 4.1	2	d, e	multiplets of diastereomeric forms
4.75	2	I	multiplets (not resolved)
7.45	2	b, c	multiplets
7.65	1	a	multiplets
7.85	1	l	two singlets of the diastereomeric forms
8.4	1	k	two singlets of the diastereomeric forms

## Mass spectrum


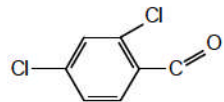
### - Operating Procedures

Instrument :	Finigan 4500	Type of analyzer :
quadrupole		
Ionization mode :	electron impact	Detection :
scan mode		
Ionizing energy :	70 eV	



### - Peak List

m / z



341	$M^+$ (not detected)
298/300	$M^+$ - $C_3H_7$
259 / 261	$M^+$ - $CH_2$ - 
191 / 193	259 - $C_5H_8$
173 / 175	
69	$C_5H_9$
55	69 - $CH_2$

**Evaluation by Competent Authorities**

1 December 2005   


### 3.5 Solubility in water including effect of pH on solubility

General Information	
<b>Title of the study:</b>	<b>Report on water solubility</b>
Project number:	AG-87 / 22P
Author:	K. Jäkel
Syngenta file number (SAM):	64250 - 2085
Name and address of testing facility:	SYNGENTA Ltd., CH-4002 Basle, Switzerland
Date of report:	November 19, 1987
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.6, OECD No. 105
Test substance:	CGA 64250 pure
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The **solubility** of the pure active ingredient in **pure water** was determined to be :

**100 mg / l at 20°C and pH 6.9**

In aqueous solution the neutral form of propiconazole is predominantly present at pH > 1.1 (pK<sub>a</sub>= 1.09). That means the pH should have no appreciable effect on the water solubility of propiconazole in the pH range 4 to 10.

#### Information on temperature effects.

Propiconazole is a non-polar organic compound of high solubility in organic media such as toluene, n-octanol and ethyl acetate, in which it is completely miscible. In contrast, propiconazole exhibits very low solubility in water. As defined in the directive, the water solubility of propiconazole was determined at a temperature of 20 °C where a value of 100 mg/litre was observed. However, due to the very low solubility Syngenta does not consider that it is relevant to determine the water solubility at either 10 or 30°C as such a temperature range will have negligible effect on the solubility of propiconazole.

Evaluation by Competent Authorities	
[REDACTED]	[REDACTED]
[REDACTED]	20 April 2007.
[REDACTED]	[REDACTED]

### 3.6 Dissociation constant

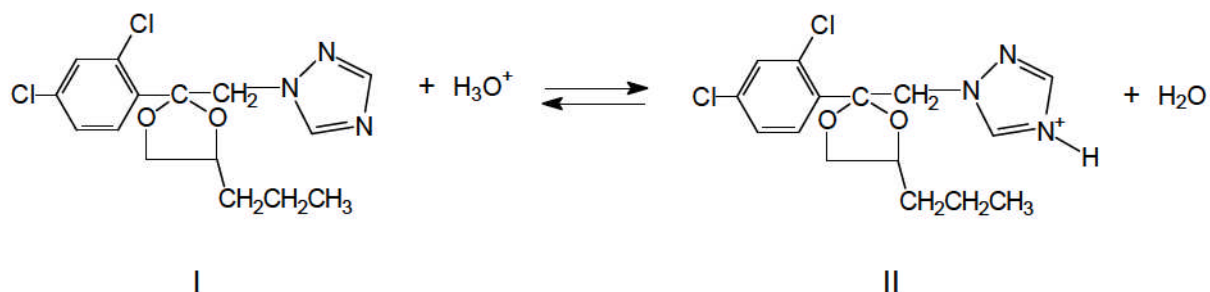
General Information	
<b>Title of the study:</b>	<b>Report on dissociation constant in water</b>
Project number:	EA 133549
Author:	K. Jäkel / J. Stulz
Syngenta file number (SAM):	64250 - 2287 / 64250 - 2455
Name and address of testing facility:	SYNGENTA Ltd., CH-4002 Basle, Switzerland
Date of report:	August 8, 1990 / October 26, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	OECD No. 112
Test substance:	CGA 64250 pure
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The **dissociation constant** of propiconazole was determined to be

$$pK_a = 1.09 \text{ at } 20^\circ\text{C}$$

The constant describes the protonation of propiconazole according to the following equation :



II shows one of the possible forms of protonated propiconazole. It can not be decided, which of the nitrogen atoms of the triazole ring is protonated.

In aqueous solutions the neutral form I is predominantly present at  $\text{pH} > 1.09$ , the protonated form II at  $\text{pH} < 1.09$ .

Evaluation by Competent Authorities
[REDACTED]
[REDACTED]

### 3.7 Solubility in organic solvents

General Information	
<b>Title of the study:</b>	<b>Report on solubility in organic solvents</b>
Project number:	20752
Author:	J. Stulz
Syngenta file number (SAM):	64250 - 2084
Name and address of testing facility:	SYNGENTA Münchwilen AG, CH-4333 Münchwilen, Switzerland
Date of report:	March 15, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	SOP 433.1.209
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
<b>Reliability indicator</b>	<b>1</b>
<b>Data Protection Claim</b>	<b>Yes</b>

#### Findings :

The **solubilities** of the technical grade active ingredient in different **organic solvents** at a temperature of 25°C were found to be :

Chemical class	Solvent	Solubility
Aliphatic hydrocarbon	n-hexane	47 g / l
Aromatic hydrocarbon	toluene	completely miscible
Halogenated hydrocarbon	dichloromethane	completely miscible
Alcohol	ethanol	completely miscible
	n-octanol	completely miscible
Ketone	acetone	completely miscible
Ester	ethyl acetate	completely miscible

#### Evaluation by Competent Authorities

[REDACTED]
[REDACTED]

### 3.8 Stability in organic solvents :

According to the TNsG on Data Requirements (current version on the ECB web site), stability in organic solvent must be stated if the active ingredient as manufactured includes organic solvent; This is not applicable to propiconazole because it does not contain organic solvents.

Evaluation by Competent Authorities	
	31 January 2011. [REDACTED]

### 3.9 Partition coefficient n-octanol / water including effect of pH

General Information	
<b>Title of the study:</b>	<b>Report on partition coefficient</b>
Project number:	AG-87 / 22P
Author:	K. Jäkel
Syngenta file number (SAM):	64250 - 2086
Name and address of testing facility:	SYNGENTA Ltd., CH-4002 Basle, Switzerland
Date of report:	November 20, 1987
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.8, OECD No. 107
Test substance:	CGA 64250 pure
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The logarithm of the **octanol / water partition coefficient** of the pure active ingredient was determined to be:

$$\log P_{ow} = 3.72 \text{ at pH } 6.6 \text{ and } 25^{\circ}\text{C}$$

#### Information on temperature effects required.

As already stated (3.5), due to the high solubility of propiconazole in n-octanol, in which it is completely miscible, and the very low solubility of the compound in water, the octanol-water partition coefficient will not be significantly affected by temperature, over the range 10 or 30 °C i.e. both parameters are essentially unchanged and therefore the log of their ratio will also effectively remain constant. Syngenta therefore considers that it is not relevant to measure the coefficient at the noted additional temperatures.

Evaluation by Competent Authorities	
	[REDACTED]
	[REDACTED]

### 3.10 Thermal Stability :

General Information	
<b>Title of the study:</b>	<b>Report on thermal stability and stability in air</b>
Project number:	20753
Author:	H. Schürch
Syngenta file number (SAM):	64250 - 2335
Name and address of testing facility:	SYNGENTA Werke Schweizerhalle AG, CH-4133 Schweizerhalle, Switzerland
Date of report:	April 18, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	OECD 113
Test substance:	CGA 64250 tech.
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The sample shows no exothermic peak between room temperature and 150°C.

Evaluation by Competent Authorities	
██████████	██████████
██████████	██████████

### 3.11 Flammability including auto-flammability

General Information	
<b>Title of the study:</b>	<b>Report on auto-flammability of liquids</b>
Project number:	PP - 94 / 10T.AFG
Author:	H. Schürch
Syngenta file number (SAM):	64250 - 2338
Name and address of testing facility:	SYNGENTA Werke Schweizerhalle AG, CH-4133 Schweizerhalle, Switzerland
Date of report:	April 18, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.10
Test substance:	CGA 64250 tech.
Batch identification:	██████████
Purity of the test substance:	██████████
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The **self-ignition temperature** of propiconazole was determined to be

430°C

**Evaluation by Competent Authorities**

20 April 2007



### 3.12 Flash point

General Information	
<b>Title of the study:</b>	<b>Report on determination of flash point</b>
Project number:	PP - 94 / 10T.FLP
Author:	H. Schürch
Syngenta file number (SAM):	64250 - 2336
Name and address of testing facility:	SYNGENTA Werke Schweizerhalle AG, CH-4133 Schweizerhalle, Switzerland
Date of report:	April 18, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.9
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings :

The **flash point** of propiconazole was determined to be

**200 °C (1013 mbar)**

Evaluation by Competent Authorities	
	20 April 2007 [REDACTED]
	[REDACTED]



### 3.13 Surface tension

General Information	
<b>Title of the study:</b>	<b>Report on surface tension of aqueous solutions</b>
Project number:	PP - 94 / 21T.SUR
Author:	M. Ryser
Syngenta file number (SAM):	64250 - 2413
Name and address of testing facility:	SYNGENTA Ltd. , CH-4002 Basle, Switzerland
Date of report:	September 19, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	OECD No. 115
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings:

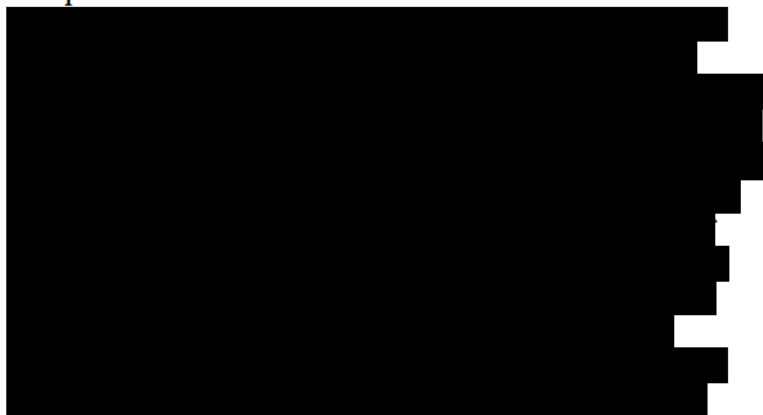
The surface tension of an aqueous suspension at 20°C by the **Wilhelmy plate method** was determined to be :

$$\delta = 46.6 - 48.4 \text{ mN / m. (filtrates of 10.0 g / l suspensions)}$$

$$\delta = 55.8 - 62.3 \text{ mN / m (filtrates of 1.0 g / l suspensions)}$$

#### Evaluation by Competent Authorities

20 April 2007.



### 3.14 Viscosity :

General Information	
<b>Title of the study:</b>	<b>Report on viscosity of liquids</b>
Project number:	PP - 96 / 32T.VIL
Author:	M. Ryser
Syngenta file number (SAM):	64250 - 3017
Name and address of testing facility:	SYNGENTA Ltd. , CH-4002 Basle, Switzerland
Date of report:	June 24, 1996
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	OECD No. 114
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings:

At 20°C : 69.630 +/- 0.379 Pa\*s at shear rate  $D = 0.10 < D < 10.0 \text{ sec}^{-1}$

At 40°C : 3.509 +/- 0.39 Pa\*s at shear rate  $D = 0.10 < D < 10.0 \text{ sec}^{-1}$

Evaluation by Competent Authorities	
[REDACTED]	[REDACTED]
[REDACTED]	[REDACTED]

### 3.15 Explosive properties

General Information	
<b>Title of the study:</b>	<b>Report on explosive properties</b>
Project number:	PP - 94 / 10T.EXP
Author:	H. Schürch
Syngenta file number (SAM):	64250 - 2337
Name and address of testing facility:	SYNGENTA Werke Schweizerhalle AG, CH-4133 Schweizerhalle, Switzerland
Date of report:	April 18, 1994
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	EEC A.14
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings:

The substance is **not considered an explosive**, as concluded from test results on :

- Thermal sensitivity (effect of a flame)
  - Mechanical sensitivity (shock)
- Mechanical sensitivity (friction) : not tested  
 The testing method is not suitable for liquids.

Evaluation by Competent Authorities	
[REDACTED]	[REDACTED]

### 3.16 Oxidizing properties

<b>General Information</b>	
<b>Title of the study:</b>	<b>Oxidizing properties (liquids) of CGA 64250 tech</b>
Project number:	81905
Author:	H. Angly
Syngenta file number (SAM):	64250 - 4299
Name and address of testing facility:	SYNGENTA Institute of Safety and Security, Testing Laboratory, Basle, Switzerland
Date of report:	March 31, 2000
Compliance with GLP:	Yes <input checked="" type="checkbox"/> No, but complies with sound scientific principles <input type="checkbox"/>
Test guidelines used:	section 34, UN 1999
Test substance:	CGA 64250 tech.
Batch identification:	[REDACTED]
Purity of the test substance:	[REDACTED]
Reliability indicator	1
Data Protection Claim	Yes

#### Findings:

The substance is not considered an oxidizing substance.

Evaluation by Competent Authorities	
1 December 2005.	[REDACTED]

### 3.17 Reactivity towards container material

The corrosion characteristics of propiconazole technical material were assessed for; tin plate, iron steel and stainless steel. For all three test materials no weight change was observed over the test period and it was therefore concluded that technical propiconazole is not corrosive to these packaging materials.

In addition, technical propiconazole is not oxidizing, not explosive, is thermally stable to at least 150 °C and has a flash point of 200 °C demonstrating its low reactivity.

Furthermore, technical propiconazole has been in large-scale manufacture and storage for in excess of twenty years without significant incident in relation to reactivity to its packaging material.

Evaluation by Competent Authorities	
1 December 2005.	[REDACTED]

