Directive 98/8/EC on the placing of biocidal products on the market.

Dossier for the inclusion of an active substance in the Annex 1

4,5-Dichloro-2-octyl-2H-isothiazol-3-one (DCOIT)

Product type 21: Antifouling products

Document III-A (A1-A3)
Study summaries – Active substance

Section A1: Applicant
Section A2: Identity
Section A3: Physical and Chemical properties

Document III-A / Section A1-A3

TABLE OF CONTENTS

Section A1 Applicant

Annex Point IIA1

1.1 Applicant

Rohm and Haas Europe Trading ApS
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DK-2100 Copenhagen Ø,
DENMARK
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Subsidiary of Rohm and Haas Company

Contact :
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06560 Valbonne
FRANCE

[redacted]
Telephone: + 33 4 93 95 53 53
[redacted]

[redacted]

1.2 Manufacturer of Active Substance

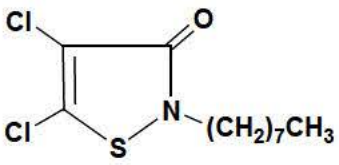
Rohm and Haas Europe Trading ApS, a wholly owned subsidiary of The Dow Chemical Company is the active substance supplier

1.3 Manufacturer of Product(s)

[redacted]

Section A2 Identity of Active Substance

Official use only

Subsection (Annex Point)		
2.1	**Common name (IIA2.1)**	There is no ISO common name for this compound. The name commonly used in the reports is DCOIT. The technical grade of the active substance can also have the trade name. Kathon™ 287T Biocide [redacted]
2.2	**Chemical name (IIA2.2)**	4,5-Dichloro-2-octylisothiazol-3(2*H*)-one (IUPAC Name) 4,5-Dichloro-2-octyl-3(2H)isothiazolone (CAS name) 4,5-Dichloro-2-octyl-2H-isothiazol-3-one (EINECS name)
2.3	**Manufacturer´s development code number(s) (IIA2.3)**	RH-25,287; RH-5287, RH-287, XB3 Technical HQ
2.4	**CAS No and EC numbers (IIA2.4)**	
2.4.1	CAS-No	64359-81-5
	Isomer	Not Applicable
2.4.2	EC-No	264-843-8
	Isomer	Not Applicable
2.4.3	Other	ENCS No. 5-6165; ECL Serial No. 93-6 (MOL)
2.5	**Molecular and structural formula, molecular mass (IIA2.5)**	
2.5.1	Molecular formula	$C_{11}H_{17}Cl_2NOS$
2.5.2	Structural formula	
2.5.3	Molecular mass	282.2 g/mol
2.6	**Method of manufacture of the active substance (IIA2.1)**	[redacted]

Section A2 Identity of Active Substance

		g/kg	g/l	% w/w	% v/v
2.7	**Specification of the purity of the active substance, as appropriate (IIA2.7)**	950 - 1000	-	95-100	-
		[redacted]			
2.8	**Identity of impurities and additives, as appropriate (IIA2.8)**	[redacted]			
	2.8.1 Isomeric composition	[redacted]			
2.9	**The origin of the natural active substance or the precursor(s) of the active substance (IIA2.9)**	[redacted]			

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	18 September 2007, revised 6 January 2009
Materials and methods	Agree with applicant's version
Conclusion	Agree with applicant's version
Reliability	-
Acceptability	Acceptable
Remarks	-

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

Subsection		Official use only
2.10.1	Human exposure towards active substance	
2.10.1.1	Production	
2.10.1.2	Intended use(s)	

Document III-A

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

i) Description of application process

[redacted]

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

ii) Workplace description

[redacted]

iii) Inhalation exposure

[redacted]

iv) Dermal exposure

[redacted]

2. Non-professional Users including the general public

[redacted]

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

2.10.2 Environmental exposure towards active substance

[redacted]

2.10.2.1 Production

[redacted]

2.10.2.2 Intended use(s)

[redacted]

Affected compartment(s):

[redacted]

Paint application and removal phase

water

[redacted]

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

sediment

air

soil

Predicted concentration in the affected compartment(s)

surface water and sediment

air

soil

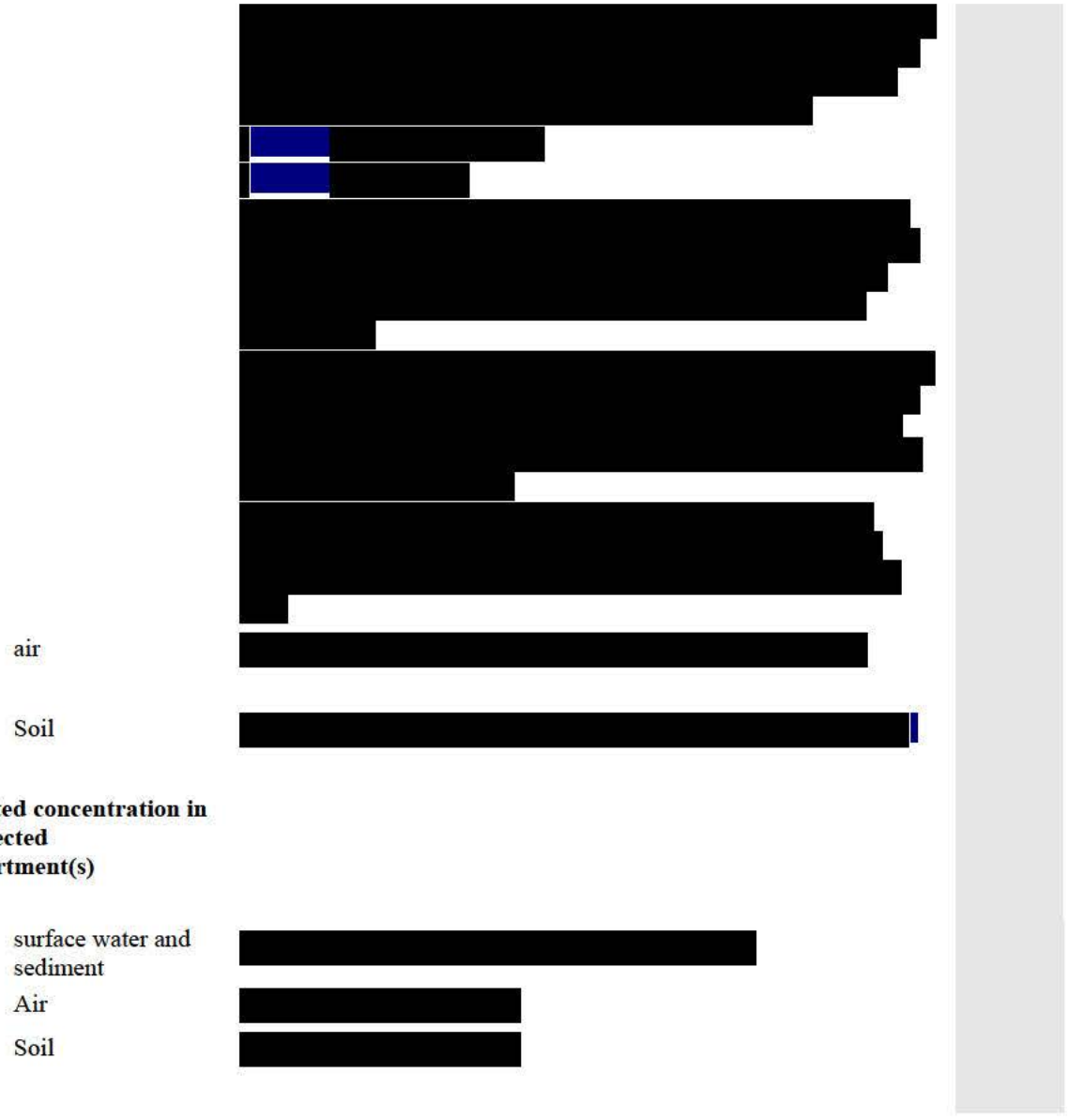
In-use phase
(Service life)

Affected compartment(s):

Water and sediments

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC



Predicted concentration in the affected compartment(s)

surface water and sediment

Air

Soil

Document III-A

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	28 January 2008
Materials and methods	-
Conclusion	Agree with applicant's version
Reliability	-
Acceptability	-
Remarks	-

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Directive 92/69/EEC, EC Method A.1 [redacted]	As defined in section 2 [redacted]	***result***: = 41.1 - 41.7°C ***pressure:*** atmospheric	None	Y	(1) Valid without restriction[1].	[redacted] Reference Type: Study	

[redacted]

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							report Year: 1994 Report date: 26 August 1994	

Section A3 Physical and Chemical Properties of Active Substance

3.1.2 Boiling point	EPA Guideline Series 63: [redacted]	As defined in section 2	**Result:** ≥ 300°C. No endothermic event was observed after the melting endotherm and up to the temperature of 300°C, at which an exothermic peak was observed, corresponding to the decomposition of the substance. RH-287 does not boil prior to its decomposition at 300°C. [redacted]	[redacted]	Y	(1) Valid without restriction[2].	Reference Type: Study report Year: 1994 Report date: 26 August 1994 [redacted]

[redacted]

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1.3 Bulk density/ relative density	EPA Guideline Series 63	As defined in section 2 [redacted]	**Result** = 1.27 g/cm^3 at 25°C. [redacted]	[redacted]	Y	(1) Valid without restriction.[3]	Reference Type: Study report Year: 1994 Report date: 26 August 1994 [redacted]	

[redacted]

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.2 Vapour pressure (IIA3.2)								
3.2.1. Vapour pressure		As defined in section 2	**Temperature:** Vapour pressures were determined at 25°C, 30°C and 35°C. **Result:** 9.8×10^{-4} Pa at 25°C 2.2×10^{-3} Pa at 30°C 4.6×10^{-3} Pa at 35°C		Y	(1) Valid without restriction.[4]	Reference Type: Study report Year: 1994 Report date: 26 August 1994	

[4] The study has been conducted in 1994 before the adoption of the Biocidal Products Directive according to a method described in Annex V of Council Directive 67/548/EEC and in accordance with the U.S. EPA principles of Good Laboratory Practice 40 CFR 160.

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	[redacted]						[redacted]	
3.2.2. Henry´s Law Constant	Calculated using the equation: Vp = k x s Where s = Saturation solubility in water at 20°C Vp = Extrapolated vapor pressure at 20°C k = Henry's Law Constant	As defined in section 2 [redacted]	**measured/calculated: result:** 3.30 x 10^{-2} Pa $m^3.mol^{-1}$ at 20°C and pH 7	[redacted]	N Calculations were not done under GLP. However individual values were obtainedunder GLP conditions.	(1) Both the vapour pressure study and the solubility study are valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							[redacted]	
3.3 Appearance (IIA3.3)								

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.3.1 Physical state	This determination was performed by visual observation with the material equilibrated at 20.0 °C using a water bath.	As defined in section 2 [redacted]	The material was found to be a solid at 20.0 °C.	None	Y	(1) Valid without restriction. [redacted]	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.3.2 Colour	This determination was performed by visual observation with the material equilibrated at 20.0 °C using a water bath.	As defined in section 2 [redacted]	The material was found to be an off-white solid at 20.0°C.	None	Y	(1) Valid without restriction. [redacted]	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.3.3 Odour	Brief nasal inhalation.	As defined in section 2 [redacted]	Moderately sweet/pungent	Determination made at 23.8°C.	Y	(1) Valid without restriction[5]	Reference Type: Study report Year: 1994 Report date: 26 August 1994 [redacted]	
3.4 Absorption spectra (IIA3.4)								

[redacted]

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.4.1 UV/VIS	The absorption spectra were obtained using a Hewlett Packard HP8452A Diode Array Spectrophotometer. Since RH-287T has such low water solubility, methanol was used as the primary solvent.	As defined in section 2 [redacted]	Concentration of RH-287 for each of the measurements was approximately 10^{-4} M. The acidic solution was in approximately 0.1N HCl. The basic solution was in approximately 0.1N NaOH. Neutral with λ=284 nm A = 1.28716 ε = 10314 $M^{-1}.cm^{-1}$ Neutral with λ=230 nm A = 0.73931 ε = 5924 $M^{-1}.cm^{-1}$ Acidic with λ=284 nm A = 1.35490 ε = 10618 $M^{-1}.cm^{-1}$ Acidic with λ=230 nm A= 0.77836 ε = 6100 $M^{-1}.cm^{-1}$ Basic with λ=227 nm A = 1.43654 ε = 13527 $M^{-1}.cm^{-1}$	[redacted]	Y	(1) Valid without restriction	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	
3.4.2 IR	The infrared spectrum was measured on a	As defined in section 2	The infrared spectrum of RH-287 shows C-H	[redacted]	Y	(1) Valid without	Reference Type: Study	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	KBr pellet at about 1% concentration of RH-287. The IR Spectrophotometer was a Nicolet FTIR model 730 equipped with Omnic E.S.P., Version 5.1b software.	[redacted]	stretches in the 2900-2800 cm^{-1} region and the carbonyl peak at 1652 cm^{-1}. Doublets at 1172-1150 cm^{-1} and 867-855 cm^{-1} are indicative of crystallinity. Conclusion: The infrared spectrum of RH-287is consistent with its chemical structure.	[redacted]		restriction	report Year: 2001 Report date: 20 December 2001 [redacted]	
3.4.3 NMR	The NMR spectrum was obtained using a chloroform-d ($CDCl_3$) solution of RH-287 at	As defined in section 2 [redacted]	Concentration of RH-287 in chloroform-d was approximately 25 % (w/w).	Both proton and carbon-13 NMR spectra were conducted to	Y	(1) Valid without restriction	Reference Type: Study report Year: 2001	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	about 25 % concentration. Tetramethylsilane (TMS) was used as an internal standard. The NMR spectrometer used was a Bruker AMX500 equipped with a 5 mm $^{1}H/^{13}C$ dual high temperature probe or 5 mm inverse detection probe.	[redacted]	Both ^{1}H and ^{13}C NMR spectra of RH-287 were conducted. The proton NMR spectrum consists of the following Chemical Shifts, δ ppm: 0.88, triplet 3H's, CH_3 group at end of octyl chain. 1.12-1.44, a series of multiplets, 10 H's, CH_2 groups in the octyl chain, excluding those H's on the 2 carbons closest to N. 1.7, quintet, 2H's, CH_2 group-second carbon removed from N on the octyl chain. 3.81, triplet, 2H's, CH_2 group next to N. The ^{13}C NMR spectrum consists of signals at the following Chemical Shifts, δ ppm: 14.1 CH_3 group at end of octyl chain.. 22.6-29.3, 5 C's, CH_2	completely characterize the structure of the active substance.			Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
			carbons in the octyl chain, excluding those 2 carbons closest to N. 31.7, CH_2 carbon, second carbon removed from N on the octyl chain. 45.1, CH_2 carbon next to N. 114.9, C-4 on the 5-membered ring. 138.3, C-5 on the 5-membered ring. 161.7, carbonyl carbon on the 5-membered ring. Conclusion: The ^{1}H and ^{13}C NMR spectra of RH-287are consistent with its chemical structure.					
3.4.4 MS	Electrospray LC-MS was used to analyze RH-287. RH-287 was dissolved in methanol and subjected to HPLC on a Hewlett Packard HPLC using a Phenomenex Spherisorb ODS1	As defined in section 2 [redacted]	About 12 mg of RH-287 were dissolved in 25 ml of methanol. The mass spectrum shows a molecular ion signal at m/z 282, consistent with active substance + H. A corresponding signal at	[redacted]	Y	(1) Valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	column at 30ºC and a mobile phase of 80% water/20% methanol. The peak of the pure active substance from the HPLC was inlet to a Micromass Quattro-SQ mass spectrometer, calibrated with a series of tetra alkyl ammonium salts in methanol. Signals were processed using COMPAQ AP200 PC with Micromass MassLnx version 3.4 software.		304 m/z is consistent with active substance plus Na ion. Presence of chlorine isotope ions at m/z 284 and 286 indicate the presence of two chlorines in the molecule. These and other signals and fragmentation patterns are consistent with the structure of the active substance. At an alternative voltage of 60 volts, the molecular ion disappears and the key fragment ions are at 172 and 174 m/z, consistent with hydrogen rearrangement resulting from the loss of the octyl chain and continued presence of two chlorines. This is further corroboration of the structure of the active substance.	[redacted]			[redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.5 Solubility in water (IIA3.5)	*including effects of pH (5-9)* Directive 92/69/EEC, EC Method A.6	As defined in section 2 [redacted]	**result:** pH = 5 2.85 mg/l at 10°C 4.26 mg/l at 20°C 6.68 mg/l at 30°C pH = 7 2.26 mg/l at 10°C 3.47 mg/l at 20°C 5.67 mg/l at 30°C pH = 9 Technically not possible. **temperature:** 10°C, 20°C and 30°C **pH:** 5 and 7 **Conclusion:** Solubility of RH-287 in water increases 2.5 times as temperature increases from 10 to 30°C. No significant effect on solubility is observed when pH increases from 5 to 7. At pH 9, RH-287	The solubility of RH-287 was tested at 10, 20, and 30 ° C. However, pH values of 5 and 7 were used instead of 5 and 9. The reason for this is that RH-287T is unstable at pH 9, especially at temperatures above 25°C. [redacted]	Y	(1) Valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
			rapidly hydrolyzes which makes the water solubility test technically not possible at this pH.					
3.6 Dissociation constant	Not Applicable	Not Applicable	**None/Not Applicable**	Scientifically unjustified. See Justification for non-submission of data.	N/A	N/A	N/A	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	These studies were performed using a method analogous to EC Method A.6, OECD 105 (water solubility). Solubility was determined in hexane and ethyl acetate at 10ºC and 30ºC. Preliminary tests were conducted to determine the solubility range. The definitive solubilities were then determined using the Shake Flask method given in EC Method A.6.	As defined in section 2 [redacted]	Solubility was determined at 10ºC and 30ºC to measure the effect of temperature on solubility. Preliminary solubility tests demonstrated that the solubility of RH-287 at 30°C in both hexane and ethyl acetate was greater than 1000g/L whereas solubility at 10°C in both solvents was much lower. Solubility tests using the Shake Flask Method and subsequent analytical measurement of the concentration of the active substance gave the following solubility results : At 30°C : Solubility in hexane greater than 704.6 g/L Solubility in ethyl acetate greater than 586.8 g/L At 10 °C	[redacted]	Y	(1) Valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
			Solubility in hexane =133.6 g/L Solubility in ethyl acetate =322.9 g/L Conclusion: There is a significant effect of the temperature on the solubility of RH-287 in both hexane and ethyl acetate.					
3.8 Stability in organic solvents (IIIA.3.2)	Not Applicable	Not Applicable	None/Not Applicable	Scientifically unjustified. See Justification for non-submission of data.	N/A	N/A	N/A	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.9 Partition coefficient n-octanol/water (IIA3.6) log Pow	*including effects of pH (5-9)* OECD Guideline 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"	As defined in section 2 [redacted]	**result: log P_{ow}** = 2.8 **temperature:** 23°C **pH:** 7	**Effect of pH on partition coefficient:** Scientifically unjustified. See Justification for non-submission of data. **Effect of Temperature on Partition Coefficient:** Scientifically unjustified. See Justification for non-submission of data.		(1) Valid without restriction.[6]	Reference Type: Study report Year: 1994 Report date: 26 August 1994 [redacted]	

[redacted]

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							[redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	CIPAC method MT 46, Differential Scanning Calorimetry,	As defined in section 2	<u>Accelerated Storage Test at 54ºC.</u> Average % Active Substance at zero time: 99.2% Average % Active Substance at 7 days: 97.3% Average % Active Substance after 14 days: 98.9% <u>Differential Scanning Calorimetry (DSC) test</u> The estimated onset temperature of decomposition was 266.1ºC. The extrapolated onset temperature of decomposition was 290.5ºC. The peak temperature of decomposition was 297.9ºC. No other exotherms were seen prior to decomposition.		Y	(1) Valid without restriction.[7]	Reference Type: Study report Year: 1994 Report date: 26 August 1994	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	[redacted]			[redacted]				
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	[redacted] EC Method A.10. [redacted] EC Method A.15 [redacted]	As defined in section 2 [redacted]	Part 1: Flammability: The analysis showed that RH-287T is not highly flammable. RH-287T melted but did not ignite under the conditions of the prescribed test. Part 2: Auto-Ignition Temperature: The auto-ignition temperature was found to be 264°C at 1012 mbar (101.2 kPa). Part 3: Relative Self-Ignition Temperature: The test showed that RH-287T does not self ignite. Conclusion: The tests conducted demonstrate that RH-287T is not a flammable substance.	[redacted]	Y	(1) Valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	[redacted] EC Method A.16.			[redacted]			[redacted]	
3.12 Flash-point (IIA3.9)	Not Applicable	Not Applicable	None/Not Applicable	Scientifically unjustified. See Justification for non-submission of data.	N/A	N/A	N/A	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.13 Surface tension (IIA3.10)	EC Method A.5, OECD 115.	As defined in section 2	**temperature:** 19ºC pH was not reported, but assumed to be about 7 as the water was double-distilled. **concentration:** 90% of saturation or ca. 3.13 ppm (3.13 mg/L). **result:** The analysis showed a surface tension of 70.8 mN/m at 19ºC		Y	(1) Valid without restriction.	Reference Type: Study report Year: 2001 Report date: 20 December 2001	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.14 Viscosity (-)	Not Applicable	Not Applicable	None/Not Applicable	See Justification for non-submission.	N/A	N/A	N/A	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.15 Explosive properties (IIA3.11)	The Non-necessity to conduct explosivity tests on RH-287T was determined using a preliminary screening using theoretical and thermodynamic data. See Justification for non-submission of data.	Not Applicable	None/Not Applicable	Scientifically unjustified. See Justification for non-submission of data	[redacted]	(1) Valid without restriction. .	Reference Type: Study report Year: 2001 Report date: 20 December 2001 [redacted]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.16 Oxidising properties (IIA3.12)	Not Applicable. Under the guidelines described in Annex IIA, III, 3.12, in cases where examination of the structural formula establishes beyond reasonable doubt that the active substance is incapable of reacting exothermally with combustible material, it is acceptable to provide such information as justification for non-determination of oxidising properties.	Not Applicable	None/Not Applicable	Scientifically unjustified. See Justification for non-submission of data.	N/A	(1) Valid without restriction.	N/A	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.17 Reactivity towards container material (IIA3.13)	Compatibility with (Reactivity towards) container material was determined by measurement of the permeability factor for RH-287T with the container type (HDPE plastic) in which the material is shipped/stored. Stability of RH-287T in the container was also determined for 27 months at ambient temperature.	As defined in section 2	The HDPE plastic permeability factor at 40°C (P_{40} Factor) was 0.68g mil/day.100in^2 (2.68 g.µm/day.cm^2) . There was no visible deterioration of the container over a 27 months period at ambient temperature. The purity of RH-287T after 27 months in the storage container was 99.0%.		Y	(1) Valid without restriction;	Reference Type: Study report Year: 1996 Report date: 1 April 1996	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
						[redacted]		

	Evaluation by Competent Authorities
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	18/9/200718, revised 6 January 2009
Comment	
Evaluation of data submitted under section A3	**3.1 Melting point, boiling point, relative density** **3.1.1. Melting point** Agree with applicant's version **3.1.2. Boiling point** Agree with applicant's version **3.1.3. Relative density/bulk density** Agree with applicant's version **3.2. Vapour pressure** Agree with applicant's version **3.2.1. Henry's Law Constant** Agree with applicant's versi **3.3. Appearance** Agree with applicant's version **3.4. Absorption spectra, and mass spectrum** Agree with applicant's version **3.5. Water solubility** Agree with applicant's version (see also justification for waiver) **3.6. Dissociation constant** See justification for waiver **3.7. Solubility in organic solvents** Agree with applicant's version **3.8. Stability in organic solvents used in b.p.** See justification for waiver **3.9 Partition coefficient *Log Pow*** Agree with applicant's version (see also justification for waiving of pH and temperature dependence) **3.10 Thermal stability** Agree with applicant's version

3.11. Flammability including autoflammability

Agree with applicant's version

3.12. Flash point

See justification for waiving

3.13 Surface tension

Agree with applicant's version

3.14. Viscosity

See justification for waiving

3.15. Explosive properties

See justification for waiving

3.16. Oxidizing properties

See justification for waiving

3.17. Reactivity towards the container

Agree with applicant's version

Section A3.5 Annex Point IIA, III. 3.5.	Water Solubility-Effect of pH	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [x]** **Scientifically unjustified [ ]** **Other justification [ ]**	
Detailed justification:	The effect of pH on water solubility was studied using pH values of 5 and 7 instead of 5 and 9. The reason for this is that RH-287 is unstable at pH 9, especially at temperatures above 25°C. The test procedure for determining water solubility using the flask method involves using an equilibration step of 1, 2, and 3 days at 40°C for determining solubility at 30°C. While RH-287 is stable at pH 7 at 40°C (Half-Life 18.7 days), it is quite unstable at pH 9 at 40°C (Half-Life 0.6 days). So values of solubility of RH-287 at pH 9 would not be meaningful. The hydrolysis study is summarized in Document IIIA Section 7.1.1.1.	
Undertaking of intended data submission [ ]	No studies are planned.	
	Evaluation by Competent Authorities	
Date	18 September 2007	
Evaluation of applicant's justification	Agree with applicant's version	
Conclusion	Agree with applicant's version	
Remarks	-	

Section A3.6 Annex Point IIIA, (-)	Dissociation constant	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [x]** **Scientifically unjustified [ ]** **Other justification [ ]**	
Detailed justification:	RH-287 (4,5-Dichloro-2-octyl-2H-isothiazol-3-one), is a covalent organic molecule that does not dissociate into ionic species. Therefore, the measurement of a dissociation constant is not applicable to this active substance.	
Undertaking of intended data submission [ ]	No studies are planned.	
	Evaluation by Competent Authorities	
Date	18 September 2007	
Evaluation of applicant's justification	Agree with applicant's version	
Conclusion	Agree with applicant's version	
Remarks	-	

Section A3.8 Annex Point IIIA, III. 2	Stability in organic solvents used in b.p. and identity of relevant breakdown products	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Detailed justification is considered as confidential information. [redacted]	
Undertaking of intended data submission [ ]	No studies are planned.	
	Evaluation by Competent Authorities	
Date	18 September 2007	
Evaluation of applicant's justification	Agree with applicant's version	
Conclusion	Agree with applicant's version	
Remarks	-	

Section A3.9 Annex Point IIA, III. 3.6	Partition coefficient n-octanol/water-Effect of pH and temperature	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Detailed justification is considered as confidential information [redacted]	

Section A3.9 Annex Point IIA, III. 3.6	Partition coefficient n-octanol/water-Effect of pH and temperature	
	[redacted]	
Undertaking of intended data submission [ ]	No studies are planned.	
	Evaluation by Competent Authorities	
Date	18 September 2007	
Evaluation of applicant's justification	Agree with applicant's version	
Conclusion	Agree with applicant's version	
Remarks	-	

Section A3.12 Annex Point IIA, III. 3.9.	Flash-point	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] Limited exposure [ ]	Technically not feasible [ ] Scientifically unjustified [x] Other justification [ ]	
Detailed justification:	RH-287T is a solid at room temperature, and it is a material of high boiling with decomposition. Therefore, its flash-point was not determined.	
Undertaking of intended data submission [ ]	No studies are planned.	
	Evaluation by Competent Authorities	
Date	18 September 2007	
Evaluation of applicant's justification	Agree with applicant's version	
Conclusion	Agree with applicant's version	
Remarks	-	