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Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	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	OECD 102 (≡ EEC A.1)	[redacted]	21.4 °C (1013.25 hPa)	The test item has a strong tendency to form a supercooled liquid.	Y	1 (valid without restrictions)	Tognucci A (2003) RCC [redacted]	X
3.1.2 Boiling point	OECD 103 (=92/69/EEC, A2)	[redacted]	no boiling point/range could be observed (1009 hPa).	Decomposition starts at 267 °C.	Y	1 (valid without restrictions)	Tognucci A (2002a) RCC [redacted]	X
3.1.3 Bulk density/ relative density	OECD 109/CIPAC MT 3 (≡ EEC A.3)	[redacted]	density : 1.040 g/cm^3 (20°C) relative density: 1.040		Y	1 (valid without restrictions)	Seal K (2002a) THOR UK [redacted]	
3.2 Vapour pressure (IIA3.2)	OECD 104 (≡ EEC A.4)	[redacted]	3.1*10^{-3} Pa (20°C) 6.1*10^{-3} Pa (25°C)	gas saturation method (extrapolated to 20°C and 25°C)	Y	1 (valid without restrictions)	Tognucci A (2002b) RCC [redacted]	
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	Calculation		3.14*10^{-3} Pa * m^3 /mol		Y	1 (valid without restrictions)	Tognucci A (2002) RCC [redacted]	

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Visual inspection		yellow liquid			4 (not assignable)	MSDS of ACTICIDE® OIT 100%	
3.3.2 Colour	Visual (Gardner) inspection		1 - 10			4 (not assignable)	MSDS of ACTICIDE® OIT 100%	
3.3.3 Odour	Olfactory inspection		mild			4 (not assignable)	MSDS of ACTICIDE® OIT 100%	
3.4 Absorption spectra (IIA3.4)								X
UV/VIS 1	UV-spectrum by HPLC/UV (DAD)	[redacted]	Absorption max. at 279 nm Extinction coefficient (279 nm): log ε = 3.92		N	4 (not assignable)	Matissek et al, Fresenius Z Anal Chem (1987) 328:108-111	X
UV/VIS 2	UV-spectrum by HPLC/UV (D AD)	[redacted]	Absorption max. at 280 nm		N	2 (valid with restrictions)	Läpple F (2006),Thor Doc 2006-FLAE-1.	
IR	no guideline stated	[redacted]	Spectral assignments [cm^{-1}]: 3070, 2920, 2850, 1610, 1470, 1310		N	2 (valid with restrictions)	Läpple F (2006),Thor Doc 2006-FLAE-1.	

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
^{1}H-NMR	no guideline stated	[redacted]	In agreement with proposed structure		N	2 (valid with restrictions)	Läpple F (2009),Thor Doc 2009-FLAE-1 referring to Diehl B (2001) Spectral Service [redacted]	
MS	no guideline stated GC/MS (EI)	[redacted]	Molecular ion M^+: m/z 213		N	2 (valid with restrictions)	Läpple F (2009),Thor Doc 2009-FLAE-1 referring to Diehl B (2001) Spectral Service [redacted]	
3.5 Solubility in water (IIA3.5)	OECD 105 (≡ EEC A.6)	[redacted]	moderately soluble pH 5: 456 mg/L at 10°C 406 mg/L at 20°C 394 mg/L at 30°C pH 7: 451 mg/L at 10°C 406 mg/L at 20°C 395 mg/L at 30°C pH 9: 483 mg/L at 10°C 433 mg/L at 20°C 448 mg/L at 30°C	flask method	Y	1 (valid without restrictions)	Geffke T (2003a) Dr. U. Noack [redacted]	X
3.6 Dissociation constant	OECD 112	[redacted]	5.2 to 6.0*10^{-4} mol/L in diluted aqueous solution	conductometric method	Y	1 (valid without restrictions)	Werle H (1993a) BioChem [redacted]	

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Subsection (Annex Point)	Method	Purity/ Specification	Results	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)								
Solubility in organic solvents 1	CIPAC MT181 CIPAC MT157 (= OECD 105) (≡ EEC A.6)	[redacted]	*In acetone* > 491.59 g/L (at 10°C) > 498.40 g/L (at 20°C) *In n-octanol* > 540.81 g/L (at 10°C) > 524.77 g/L (at 20°C)	Simplified shake-flask method OIT was completely soluble in acetone and n-octanol at a ratio of 1:1. Therefore, the solubility in these solvents must be above the values as determined analytically.	Y	1 (valid without restrictions)	Kühne M (2010i) Harlan Laboratories Ltd. [redacted]	
Solubility in organic solvents 2	Statement			OIT is marketed in various b.p. containing organic solvents. Thus, it is soluble for example in propylene glycol (ACTICIDE® 45) and 2,2,4-trimethyl-pentane-1,3-diol isobutyrate (= Texanol) (ACTICIDE® DW).	N	4 (not assignable)		X

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)	Stable in the solvents used in b.p. as mentioned in 3.7.2. The shelf live of these b.p. is up to 2 years.							X

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.9 Partition coefficient n-octanol/water (IIA3.6)								X
log Pow 1	OECD 117 (≡ EEC A.8)	[redacted]	log $P_{o/w}$: pH 7: 2.95 (10°C) pH 7: 2.92 (20°C) pH 7: 2.93 (30°C) pH 5: 2.92 (20°C) pH 7: 2.92 (20°C) pH 9: 2.94 (20°C)	HPLC-method	Y	1 (valid without restrictions)	Seal K (2002b) THOR UK, RS/01/020,	
log Pow 2	OECD 117 (≡ EEC A.8)	[redacted]	log $P_{o/w}$ = 2.5 (20°C)		Y	1 (valid without restrictions)	Toggnucci A (1998) RCC 704711,	
log Pow 3	OECD 107 (≡ EEC A.8)	[redacted]	log$P_{o/w}$ = 3.42	ACTICIDE 45-TGAI	Y	2 (valid with restrictions)	Werle H (1993b) BioChem 925040174 H	
log Pow 4	Calculation	[redacted]	log$P_{o/w}$ > 3.1	Based on a solubility of OIT in n-octanol of >524.8 g/L (at 20°C) and a solubility of OIT in water of 0.406 g/L (at 20°C).	Y	1 (valid without restrictions)	Kühne M (2010k) Harlan Laboratories Ltd. C76752	
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	OECD A113 CIPAC MT 46.1.3	[redacted]	initial content: 99.9 % content after storage at 54°C: 98.9%	accelerated storage test (for 14 days at 54±2°C in a glass bottle)	N	2 (valid with restrictions)	Bleif J (2000) THOR, 2001-BLF	X

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	Statement concerning EEC A. 12 and EEC A 13 (flammability in contact with water and pyrophoric properties)		EEC A10 only applies to solids	Due to the chemical structure of OIT and based on long lasting experience it can be stated that OIT is not flammable in contact with water and has no pyrophoric properties. This has been experienced over years when the product is handled and used as preservative in aqueous systems. According to the TNsG on data requirements, pg. 30, test A12/A13 can be omitted if experience in use indicates that negative results would be obtained.	N	4 (not assignable)		
	EEC A15 (auto-ignition)	[redacted]	Auto ignition temperature: 330°C	Mean of three determinations	Y	1 (valid without restrictions)	Paulus J. (2007a) LAUS 07061303G 962	

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.12 Flash-point (IIA3.9)		[redacted]						X
Flash point 1	IP 170 / ISO 13 736 (acc to Abel)	[redacted]	no flash point was detected up to 70°C		N	2 (valid with restrictions)		
Flash point 2	EEC A.9 (Pensky-Martens)	[redacted]	156.5°C		Y	1 (valid without restrictions)	Paulus J. (2007b) LAUS 07061303G 964	
3.13 Surface tension (IIA3.10)	EEC A.5 / OECD 115	[redacted]	35.97 mN/m at 20.1°C surface active	90% saturation concentration	Y	1 (valid without restrictions)	Paulus J. (2007c) LAUS 07061303G 960	
3.14 Viscosity								
Viscosity 1	OECD 114 DIN 51 562	[redacted] (exact purity not stated in the report [redacted] is derived from the product specification)	dynamic viscosity: 78.95 mPa s (20°C) kinematic viscosity: 76.48 mm^2/s (20°C) 29.02 mm^2/s (40°C)	Capillary Method	Y	1 (valid without restrictions)	Rueb B (1995) THOR, 9503-BR-63/18,	

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Viscosity 2	OECD 114 DIN 53 019	[redacted]	dynamic viscosity: 39 – 45 mPa s (30°C) 14 – 15 mPa s (50°C)	Rotational viscometer Note: only one spindle/vessel combination was tested; at 20°C the test item was in the solid state, therefore a higher temperature had to be chosen	N	2 (valid with restrictions)	Van der Baan-Treur (2004) NOTOX, 406261	
3.15 Explosive properties (IIA3.11)	EEC A14 (statement)		not explosive From the chemical structure of OIT it can be derived that OIT does not possess explosive properties since it contains none of the structural alerts for explosive properties as listed in the TNsG on Product Evaluation.		N	4 (not assignable)		
3.16 Oxidising properties (IIA3.12)	EEC A17 (statement)		not oxidising From the chemical structure of OIT it can be derived that OIT possesses no oxidising properties since it contains none of the structural alerts for oxidising properties as listed in the TNsG on Product Evaluation.		N	4 (not assignable)		

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Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.17 Reactivity towards container material (IIA3.13)	OIT has been stored in a range of containers (such as plastic bags in metallic containers and plastic containers). No interaction between the active ingredient and the container materials has been observed since production and marketing started. Based on results in use and examination of the chemical structure, there are considered to be no problems with reactivity of the active substance towards the container materials used.							

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22/10/2009
Materials and methods	It should be noted that the dossier for OIT PT 8 was submitted prior to 01/09/2013. Hence the data were assessed against the data requirements and guidelines for directive 98/8. None of the chemistry data requirements are associated with critical areas of concern that must be addressed as a result of the implementation of regulation 528/2012. The Applicant's version is considered to be acceptable with the following comments: **3.1.2 Melting/freezing point** Method: 92/69/EEC Method A.1 (DSC), OECD 102 **3.1.3 Relative Density** Method: 92/69/EEC Method A.3 (Pycnometer), OECD 109/CIPAC MT3 **3.4 Absorption spectra** UV-VIS 1 – This is a published paper and no purity information is provided hence the reliability value of 4. The other studies are given a reliability of 2 as they are not to GLP however they are of sufficient standard to confirm the structure. It is noted that the absorption at different pH has not been assessed. These data should be provided post approval of the active, but prior to the date of entry into force. No absorbance above 290 nm occurred. **3.5 Water solubility** Method : 92/69/EEC Method A.6 (Modified flask method), OECD 105 Sample analysis by HPLC (UV detection @282nm) The study used water buffered to pH5, 7 & 9 but did not measure the solubility of the substance in unbuffered water. A second study was submitted where the shake flask method was used to measure the solubility of the substance (purity 90%) in unbuffered water. The result of 525.2 mg/l was obtained. The average pH of the saturated solution was 3.4. Samples were analysed by HPLC (UV detection @ 275nm). Reference Werle H (1992) BioChem 925040174G. **3.6 solubility in organic solvents** The solubility in two organic solvents of different polarity have been tested. The results demonstrate that OIT is readily soluble in both solvents. This statement on the solubility from the applicant should be deleted. **3.8 Stability in organic solvents used in b.p. and identity of relevant**

	breakdown products There are no solvents in the technical material as manufactured. **3.9 Partition coefficient** Method 1: 92/69/EEC Method A.8 (HPLC method), OECD 117 Method 2: 92/69/EEC Method A.8 (HPLC method), OECD 117 Method 3: 92/69/EEC Method A.8 (Shake flask method), OECD 117 Analysis by HPLC UV detection (275nm) According to the test method guideline neither the shake flask nor the HPLC methods are applicable for the determination of log Pow of surface active substances. The applicant has therefore provided an estimation (by calculation) of the partition coefficient based on the individual n-octanol and water solubilities. The result is acceptable. The other results should be deleted as the test methods used were inappropriate for the active. The result demonstrates that OIT has the potential to be fat soluble. Results 1-3 can be deleted as they have used inappropriate test methods. Only result 4 (by calculatio) is valid. **3.10 Thermal stability** Method: OECD 113, CIPAC MT46 The study was not conducted to GLP but meets the requirements of DIN EN ISO 9001. **3.12 Flash Point** Delete flash point 1
Conclusion	N/A
Reliability	1 There are a number of reliability indicators presented within this summary and it is therefore difficult for the UK CA to agree with one figure. However, overall the UK CA finds all data presented, and studies performed, to be reliable and scientifically accurate. Therefore, for completeness of the document the reliability indicator is 1.
Acceptability	Acceptable
Remarks	

	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	