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	OECD 102 (≡ EEC A.1)	Batch XXXX, purity XX%	**result: 233 to 236 °C pressure: atmospheric**	-	Y	1	Xxxxxxx, XXXXx	x
3.1.2 Boiling point	Not required, the active substance is a solid with a melting point range of 233 to 236 °C.							x
3.1.3 Bulk density/ relative density	OECD 109/CIPAC MT 3 (≡ EEC A.3)	Batch XXXX, purity XX%	**Relative density = 1.36 g/mL**	Test conducted at 25 °C.	Y	1	Xxxxxxx, XXXXx	x
3.2 Vapour pressure (IIA3.2)	OECD 104 (≡ EEC A.4)	Batch XXXX, purity XX%	**result: <1.3 x 10^{-5} Pa**	Test conducted at 22.6 °C.	Y	1	Xxxxxxx, XXXXx	x
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	Calculation	-	**measured/calculated: result: <1.5 x 10^{-3} Pa.m^3.mol^{-1}**	Calculated from vapour pressure of <1.333 x 10^{-5} Pa and water solubility of <4.8 mg/L (limit value).	Y	1	Xxxxxxx, XXXXx	x
3.2.1 Henry´s Law Constant	Calculation		**0.018 Pa.m^3.mol^{-1}**	Calculated from vapour pressure of 1.3 x 10^{-5} Pa and water solubility of 0.39 mg/L	N	2		x

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3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Visual	Batch XXXX, purity XX%	**Powder**	-	Y	1	Xxxxxx, XXXXx	
3.3.2 Colour	Visual (Munsell colour system)	Batch XXXX, purity XX%	**Yellow 2.5y (9/2)**	-	Y	1	Xxxxxx, XXXXx	
3.3.3 Odour	Olfactory - ASTM D1292-80	Batch XXXX, purity XX%	**Odourless**	-	Y	1	Xxxxxx, XXXXx	
3.4 Absorption spectra (IIA3.4)								
UV/VIS	-	Not stated	**All spectra are consistent with the structure of the active substance**	-	N	2	Xxxxxxx, XXXX	x
IR	-	Not stated		-	N	2	Xxxxxxx, XXXX	x
NMR	Proton and 13C NMR	Not stated		-	N	2	Xxxxxxx, XXXX	x
MS	APCI ± HPLC-MS	Not stated		-	N	2	Xxxxxxx, XXXX	x

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3.5 Solubility in water (IIA3.5)								
Water solubility 1	OECD 105 (≡ EEC A.6)	Batch XXXXXXXXX X, purity XX%	**result: <0.02, <0.02, <0.10 mg/L** **temperature: 20°C** **pH: 4, 7, 9** **Limit value <4.8 mg/L (MilliRo water)**	Shake flask method.	Y	1	Xxxxxx, XXXXx	x
Water solubility 2	OECD 105 (≡ EEC A.6)	Batch XXXX, purity XX%	**result: 0.39 mg/L** **temperature: 25°C** **pH: not stated**	Column elution method.	Y	2	Xxxxxxx, XXXXx	x
3.6 Dissociation constant (-)	Due to the low water solubility of difethialone, the test item is not considered ionisable and attempts to determine this are impractical.							
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	OECD 105 CIPAC MT 181	Batch XXXX XXXXXX, purity XX%	**Dichloromethane** **Hexane**	-	Y	2	Xxxxxx, XXXXx	x
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)	Not applicable because the active substance as manufactured does not include an organic solvent and is not formulated in organic solution in the biocidal product.							

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 1	OECD 117 (≡ EEC A.8)	Batch XXXX XXXXXX, purity XX%	**result: log Pow = 6.29 temperature: ambient pH: 7.3**	HPLC method.	Y	2	Xxxxxx, XXXXx	x
log Pow 2	OECD 107 (≡ EEC A.8)	Batch XXXXXX, purity X%	**result: log Pow = 5.00 temperature: 23 °C pH: not stated**	Shake flask method.	Y	2	Xxxxx, XXXxx	x
	Due to the low water solubility of difethialone, the test item is not considered ionisable. Therefore investigation of the pH effect on the partition coefficient is not necessary.							
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	OECD A113	Batch XXXX XXXXXX, purity XX%	**Stable at room temperature**	Tested using differential scanning calorimetry.	Y	1	Xxxxxxx, XXXX	
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	EEC A10 (flammability of solids)	Batch XXXX XXXXXX, purity XX%	**Not flammable**	-	Y	1	Xxxxxxx, XXXX	x
	EEC A16 (auto-ignition)	Batch XXXX XXXXXX, purity XX%	**Not auto-flammable**	-	Y	1	Xxxxxxx, XXXX	x
3.12 Flash-point (IIA3.9)	Not required for a solid active substance.							

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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)	Not required because the water solubility of the active substance is below 1 mg/L.							
3.14 Viscosity (-)	Not applicable because the active substance is a solid.							
3.15 Explosive properties (IIA3.11)	EEC A14	Batch XXXX XXXXXX, purity XX%	**Not explosive**	Tested for explosivity due to heat, mechanical shock and friction.	Y	1	Xxxxxxx, XXXX	
3.16 Oxidising properties (IIA3.12)	EEC A17	Batch XXXX XXXXXX, purity XX%	**Not oxidising**	-	Y	1	Xxxxxxx, XXXX	
3.17 Reactivity towards container material (IIA3.13)	Difethialone 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 in the past 20 years of production. 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 material.							x
	Evaluation by Competent Authorities							
	EVALUATION BY RAPPORTEUR MEMBER STATE							
Date	18 January 2005, revised 28 September 2006							
3.1.1 Melting point	28 September 2006: Method used was the block method as described in OECD 102							
3.1.2 Boiling point	28 September 2006: No boiling point has been determined. Taking into account the high melting point of difethialone and that handling of products containing difethialone takes place at room temperature data on the boiling point are not considered essential to provide information of scientific relevance for the use in any part of the risk assessment nor are they needed to ensure safe handling of the a.s. or the products as such.							
3.1.3 Bulk density/relative density	28 September 2006: Method used was the Pycnometer method as described in OECD 109 The given value refers to the density and not to the relative density.							

3.2 Vapour pressure	In the Xxxxxxx study (OECD104) the vapour pressure is not detectable because the amount of difethialone recovered was below the chemical analytical detection limit of the method used. The estimated vapour pressure was therefore based on the 2 * detection limit giving an estimated vapour pressure of $<1.333x10^{-5}$ Pa. Use of detection limit ($<1.333x10^{-5}$ Pa) as endpoint is not satisfactory. Tomlin, C. (1997) refer to a measurement of VP=$5.55x10^{-7}$ mmHg=$7.4x10^{-5}$ Pa, however without a being able to locate the primary source of this data, and evaluate its quality the data of Xxxxxxx (XXXX) will be retained for risk assessment purposes. The vapour pressure is not a critical factor in the risk assessment and it is therefore not justified to ask for a study giving a more precise determination of the vapour pressure. 28 September 2006: Method used was the gas saturation method as described in OECD 104 (test temperature 22.6°C)	
Conclusion	The vapour pressure = $1.333x10^{-5}$ Pa is used in the risk assessment.	
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	As it has been concluded that the water solubility value of 0.39 mg/l (Xxxxxxx, XXXX) is the most representative value, there is need to recalculate the Henry's Law constant. Therefore using the vapour pressure of $1.333x10^{-5}$ and the water solubility of 0.39 mg/l from Xxxxxxx, XXXX (=$7.2x10^{-4}$ mol)) results in a Henry's Law constant of H=0.018 Pa m^3/mol. 28 September 2006: The value of 0.018 Pa.m^3.mol^{-1} will be used for risk assessment	
Conclusion	The Henry 's Law constant used should be H=0.018 Pa m^3/mol, logH=-1.74	
3.4 Adsorption spectra **(IIA3.4)**	NMR: The total number of hydrogen from the integrals should theoretically be 23 but was 33. LC-MS: Retention time on chromatogram: The compound should have more retention to be able to extinguish it from the void volume. Difethialone is a relatively large molecule and gives complex spectra. With the information available from the existing spectra it was not entirely possible to conclude which carbon gave which signal. More information might be necessary before the knowledge over its structure becomes unambiguously clear. However, in all likelihood the spectra available represent difethialone clearly.	
Conclusion	All spectra are in all likelihood consistent with the structure of the active substance	
3.5 Solubility in water	The study of Xxxxxx XXXX gives a water solubility of <4.8 mg/l while the study of Xxxxxxx XXXX gives a solubility of 0.39 mg/l. In the study of Xxxxxx the analytical method applied was not able to detect concentrations below 4.8 mg/l. This is in contrast to the study of Xxxxxxx (XXXX) where a total of 14 determinations were made during a time series (equilibrium times from zero minutes to 24 hours. Maximum observed concentration was 0.97 mg/l measured after 1 hour. The value of 0.39 mg/l is the mean of the latter 5 measuring points observed in the period 20-24 hours. The standard deviation around the mean is 0.09 mg/l. 28 September 2006: The flask method (Xxxxxxx XXXX) is not applicable for substances with a water solubility of < 0.02 g/l. Therefore the test result is considered to be invalid and the reliability indicator is changed to 3. The value of 0.39 mg/l (Xxxxxxx XXXX) will be used for risk assessment.	
Conclusion	A water solubility of 0.39 mg/l is used in this risk assessment.	

3.7 Solubility in organic solvents	28 September 2006: Solubility in dichloromethane was conducted according to CIPAC MT 181 method. For hexane the shake flask method described in OECD 105 was used. Test temperature was 20°C for dichloromethane (test concentration 10 to 14 g/l). Regarding hexane the test temperature of 20°C was followed by a storage period at 30°C (24, 48 and 72 hours). Test concentration for hexane was 0.2 g/l.	
3.9 Partition coefficient n-octanol/water	The study of Xxxxxxx XXXX gives a Log Pow of 6.29 while the shale flask method of Xxxxxxx XXXX gives a log Pow=5.0 The study of Xxxxxxx XXXX indicates large problems with correct detection of the concentration of difethialone in the water phase. Although 31 runs were performed one can assume that results might be skewed. Therefore the study of Xxxxxxx XXXX is believed to give the most reliable value even though the test compound is outside the range of the standard compounds used. The log Pow=6.29 is comparable to an experimental value of Log Pow= 5.9 referred to by Tomlin, C (1997). Reference: Tomlin , C. (1997) The Pesticide Manual. Tenth edition. The Royal Society of Chemistry. Pp. 1344. ISBN 0-948404-79-5. <u>QSAR estimation of BCF:</u> A log Pow of 6.29 gives BCF fish =39974 l/kg (TGD calculation) 28 September 2006: The shake flask method (Xxxxxxx XXXX) is not applicable for substances with a log Pwo-value>4. Therefore the value is regarded as invalid and the reliability indicator is changed to 3. The log Pow of 6.29 (Xxxxxxx XXXX) will be used for risk assessment.	
Conclusion	Log Pow =6.29 (BCF fish = 39974 l/kg, calculated)	
3.11 Flammability, including auto-flammability and identity of combustion products	28 September 2006: The result on flammability is “not highly flammable” 28 September 2006: The result on auto-flammability is “no self ignition at temperatures up to the melting point (233 to 236°C).”	
3.17 Reactivity towards container material (IIA3.13)	28 September 2006: Packing, storage and transport of difethialone is done in plastic bags, placed in cartoon drums, which are UN-accredited in accordance with transport legislation. This drum is made out of Natron-kraftliner coated with PE in sic layer. And one inside layer made of aluminium-PE. The top and bottom of the drum are made out of galvanized steel sheet and the closure is a galvanized adaptor ring with rubber sealing. However, difethialone can be packed, stored and transported in many different packaging materials, namely multi layer of paper, cartoon, plastics (e.g. polypropylene, polyethylene, polyethyleneterephthalat). The list of materials can not be considered as exhaustive as difethialone has no known physical-chemical properties which would support the assumption that any reactivity with container material would take place.	