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	EEC Directive 92/69 EEC A.1 (DSC)	Not indicated	**< - 90 °C** During a DSC experiment, the substance was cooled down to -90 °C without solidification.	According to the TNsG on data requirements "Usually the freezing point of liquid substances should be determined if above -20°C. An indication that no freezing has occurred during preliminary tests is also acceptable." Therefore, the applicant considers the performed study as sufficient to cover this data requirement and the performance of a GLP test not to be necessary.	N	[redacted]	112-002 A3.1.1/01	x

[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
3.1.2 Boiling point	EEC Directive 92/69 EEC A.2 EPA OPTTS 830.7220 EPA subdivision D series 63-6	[redacted] purity: 99.8%	- exothermic effect at ca. 141 °C (probably decomposition) **- endothermic effect slightly below 300 °C (metastable boiling point)**	Differential Scanning Calorimeter (DSC) was used	Y	[redacted]	112-001 A3.1.2/01	x
3.1.3 Bulk density/ relative density								
rel. density	EEC Directive 92/69 EEC A.3 OECD 109 EPA OPTTS 830.7300 EPA subdivision D series 63-7	[redacted] purity: 99.8%	**0.998 (at 20°C +/- 0.5 °C)**	Measured with a pycnometer	Y	[redacted]	113-001 A3.1.3/01	x
3.2 Vapour pressure (IIA3.2)	EEC Directive 92/69 EEC A.4 (static technique). OECD 104 EPA OPTTS 830.7950 EPA subdivision D series 63-9	[redacted] purity: 99.8%	**0.15 +/- 0.01 Pa at 20°C** **0.22 +/- 0.01 Pa at 25°C**	None. Calculated via $\ln p/T^{-1}$ curve: ln p [Pa] = -6874.6/T[K] + 21.548	Y	[redacted]	115-001 A3.2/01	

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
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	Calculated parameter	Not applicable	**0.000461 Pa m^3 mol^{-1} (20°C)**	Calculated with reference to: Aqueous solubility = 70 g/L (20°C) (see 3.5) Vapour pressure = 0.15 Pa (20°C) (see 3.2) Molar weight = 215.29 g/mol	N	[redacted]	None	
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	EPA OPPTS 830.6303 EPA subdivision D series 63-3	[redacted] purity: 99.8%	**Liquid (at 21°C)**	None	Y	[redacted]	111-001 A3.3.1/01	
3.3.2 Colour	EPA OPPTS 830.6302 EPA subdivision D series 63-2	[redacted] purity: 99.8%	**Clear and colourless (at 21°C)**	None	Y	[redacted]	111-001 A3.3.1/01	
3.3.3 Odour	EPA OPPTS 830.6304 EPA subdivision D series 63-4	[redacted] purity: 99.8%	**No characteristic odour (at 21°C)**	None	Y	[redacted]	111-001 A3.3.1/01	

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 Absorption spectra (IIA3.4)								
3.4.1 UV/VIS	OECD 101 EPA OPTTS 830.7050	[redacted] purity: 99.8%	**No absorbance maxima were observed under neutral (900 – 200nm), acidic (900 – 205nm) and alkaline conditions (900 – 220nm) (25°C +/ 0.5 °C)**	None	Y	[redacted]	117-001 A3.4.1/01	
	No guideline mentioned	Not mentioned	**The respective spectra confirms the molecular structure of IR3535**	None	N	[redacted]	117-002 A3.4.1/02	
	50,08 mg in 50 mL water. 200 – 800 nm. Slit 2 nm. Intervall 0.1 s. Stepsize 0.5 nm. Base line: water. Cell length: 1 cm.	[redacted] purity: 99.4%	**The UV-VIS spectrum shows only the flank of the absorption bands due to n → π* transitions of the ester and amide group below 250 nm.**	None	N	[redacted]	117-003 A3.4.1/03	
3.4.2 IR	No guideline mentioned	Not mentioned	**The respective spectra confirms the molecular structure of IR3535**	None	N	[redacted]	117-002 A3.4.1/02	
	FT-IR Spectroscopy, Bruker Vector 22, spectral resolution 2 cm^{-1}, 32 scans, KBr-pellet	[redacted] purity: 99.4%	**The respective spectrum confirms the molecular structure of IR3535**	None	N	[redacted]	117-003 A3.4.1/03	
3.4.3 NMR	No guideline mentioned	Not mentioned	**The respective spectra confirms the molecular structure of IR3535**	None	N	[redacted]	117-002 A3.4.1/02	

[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
	Bruker DPX300; samples in d_6-DMSO. ^{1}H: 353K, 32 scans ^{13}C: 393K, 1024 scans	[redacted] purity: 99.4%	**The respective spectra confirm the molecular structure of IR3535**	None	N	[redacted]	117-003 A3.4.1/03	
3.4.4 MS	No guideline mentioned	Not mentioned	**The respective spectra confirms the molecular structure of IR3535**	None	N	[redacted]	117-002 A3.4.1/02	
	EI-MS. Waters "Autospec" at 140 °C.	[redacted] purity: 99.4%	**The respective spectrum confirms the molecular structure of IR3535**	None	N	[redacted]	117-003 A3.4.1/03	
3.5 Solubility in water (IIA3.5)								
Water solubility	EEC Directive 92/69 EEC A.6 OECD 105 EPA OPTTS 830.7840 EPA subdivision D series 63-8	[redacted] purity: 99.8%	**70 g/L at 20.0°C +/- 0.5°C**	Shake flask method, using distilled water, without pH control was used.	Y	[redacted]	114-004 A3.5/01	

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
Water solubility	EEC Directive 92/69 EEC A.6	[redacted] purity: 99.9%	**pH 5: 69.92 g/L pH 7: 56.72 g/L pH 9: 68.0 g/L (t 20°C +/- 1°C)**	Shake flask method was used. At pH 9 the test item was unstable due to hydrolysis. The given result is assumed to reflect the equilibrium between hydrolysis and solubility.	Y	[redacted]	114-005 A3.5/02	
3.6 Dissociation constant (-)			**Not applicable**	The test item is not ionisable and therefore could not dissociate in water. A detailed justification is provided in the "Evaluation by Competent Authorities" table at the end of this document.				
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	EPA subdivision D series 63-8	[redacted] purity: 99.8%	**Acetone >1000g/L Ethyl acetate >1000g/L Dichloromethane >1000g/L n-Heptane >1000g/L Methanol >865g/L p-Xylene >1000g/L**	None	Y	[redacted]	114-001 A3.7/01	

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
			(at room temperature)					
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)			**Stable in common organic solvents**	Additional information confirming the stability of IR3535® in the organic solvent ethanol that is mostly used in formulation is given in Doc-no.: 114-006 This document contains confidential information and therefore notifier requests a confidential treatment of this document.	Y	[redacted]	114-001 A3.7/01 114-006 A3.8/01	
3.9 Partition coefficient n-octanol/water (IIA3.6)								
log Pow	EEC Directive 92/69 EEC A.8 OECD 117 EPA OPTTS 830.7570 EPA subdivision D series 63-11	[redacted] purity: 99.8%	**log Pow : 1.7 (at: 23-24°C)**	HPLC method As the test item is not ionisable, investigation on the pH effect on the partition coefficient is not necessary.	Y	[redacted]	114-003 A3.9/01	X

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]		
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	CIPAC MT 46 EPA OPTTS 830.6313 EPA subdivision D series 63-13	[redacted] purity: 99.8%	**The test substance is stable at 54 °C for 14 days. No exothermal decomposition was observed up to 141 °C, please refer to 3.1.2**	No changes in its purity was measured. No breakdown products were identified.	Y	[redacted]	141-001 A3.10/01	
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)								
Flammability			**Not applicable**	According to TNsG the flammability of substances which are solids, gases or substances which evolve highly flammable gases must be determined. This is not the case for IR3535® a testing is therefore not necessary.				
Auto-flammability			**Not auto-flammable**	No exothermal decomposition was				

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
				observed up to 350 °C, please refer to 3.1.2				
3.12 Flash-point (IIA3.9)	EEC Directive 92/69 EEC A.9 DIN EN22719 EPA OPTTS 830.6315 EPA subdivision D series 63-15	[redacted] purity: 99.8%	**159°C**	Pensky Martens closed cup	Y	[redacted]	142-001 A3.12/01	
3.13 Surface tension (IIA3.10)	EEC Directive 92/69 EEC A.5	[redacted] purity: 99.7%	**59.6mN/m at 20.0°C ± 0.5°C (n=3)**	Ring method concentration of test solution: 1 g/L aqueous solution	Y	[redacted]	116-002 A3.13/01	
3.14 Viscosity (-)	OECD 114 DIN 53019 Teil 1 EPA OPTTS 830.7100 EPA subdivision D series 63-18	[redacted] purity: 99.8%	**Viscosity: 14 – 22 mPa.s (at 20°C ± 0.5°C)** **Viscosity: 16 mPa.s at (40°C ± 0.4°C)**	Rotational Viscometer	Y	[redacted]	116-001 A3.14/01	
3.15 Explosive properties (IIA3.11)	EEC Directive 92/69 EEC A.14	Not applicable	**Not explosive**	The compound does not contain reactive groups that indicates explosive properties.	N	[redacted]	141-003 A3.15/01	
	Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods,	Not applicable	**Not explosive** Based on a screening of the molecular structure of IR3535 according to	A detailed justification is provided in the "Evaluation by Competent	N	[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
	Manual of Tests and Criteria"(4th revised edition)		Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria", it can reasonably be concluded that IR3535 is not explosive.	Authorities" table at the end of this document.			[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)	EEC Directive 92/69 EEC A.17	Not applicable	**Not oxidising**	The compound does not contain reactive groups that indicates oxidising properties.	N	[redacted]	141-003 A3.15/01	
	Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria"(4th revised edition) and supplement to A.17	Not applicable	**Not oxidising** Based on the criteria set out in the Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria"(4th revised edition) and the criteria set out in the supplement to A.17* method as provided by the UK Health and Safety Executive (http://www.hse.gov.uk/nonsnonsa17.htm) it can reasonably be concluded that IR3535 is not oxidising.	A detailed justification is provided in the "Evaluation by Competent Authorities" table at the end of this document.	N	[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
3.17 Reactivity towards container material (IIA3.13)	EPA OPTTS 830.6313 EPA subdivision D series 63-13	[redacted] purity: 99.8%	**No significant change in appearance and/or decrease in concentration was observed after exposition of IR3535® to iron/iron ions and copper/copper ions for 14 days at 20°C ± 1°C and 54°C ± 1°C, respectively.**	None	Y	[redacted]	146-001 A3.17/01	
	EPA OPTTS 830.6317 EPA OPTTS 830.6320	[redacted] purity: 99.8 %	**The commercial storage container (HDPE) does not change physically during a 1 year storage period at warehouse conditions.**	None	Y	[redacted]	146-003 A3.17/02	

Evaluation by Competent Authorities	
	MELTING POINT (3.1.1)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	[redacted]
Conclusion	
Reliability	
Acceptability	
Remarks	
	EVALUATION BY RAPPORTEUR MEMBER STATE

Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
1.1	*Evaluation by Rapporteur Member State*
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]

Evaluation by Competent Authorities	
	BOILING POINT (3.1.2)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	
Conclusion	[redacted]
Reliability	
Acceptability	
Remarks	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]

Evaluation by Competent Authorities	
	DISSOCIATION CONSTANT (3.6)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	[redacted]

Conclusion	
Reliability	
Acceptability	
Remarks	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]

Evaluation by Competent Authorities	
	PARTITION COEFFICIENT N-OCTANOL/WATER (3.9)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	[redacted]
Conclusion	
Reliability	
Acceptability	

Remarks	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]

Evaluation by Competent Authorities	
	EXPLOSIVE PROPERTIES (3.15)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	[redacted]

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[redacted]	[redacted]

[redacted]

Conclusion [redacted]

Reliability [redacted]

Acceptability

Remarks

EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]

Evaluation by Competent Authorities	
	OXIDISING PROPERTIES (3.16)
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	[redacted]
Evaluation of applicant's justification	[redacted]
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]
	COMMENTS FROM INDUSTRY
Date	[redacted]
Results and discussion	[redacted]

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Conclusion	[redacted]
Reliability	[redacted]
Acceptability	
Remarks	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	[redacted]
Evaluation of applicant's justification	
Conclusion	[redacted]
Acceptability	[redacted]
Remarks	[redacted]