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24-Epibrassinolide

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Rapporteur Member State: Austria

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B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.1. MELTING POINT AND BOILING POINT						
Melting, freezing or solidification point **B.2.1/01**	EEC A.1 OECD 102	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	Melting point: 254.6–258.2 °C	Acceptable	Y	Gao, J. (2015)
Boiling point **B.2.1/02**	EEC A.2 OECD 103	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	No boiling or decomposition of the test item could be observed up to 400 °C	Acceptable	Y	Gao, J. (2015)
Decomposition / Sublimation temperature **B.2.1/03**	EEC A.2 OECD 103	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	No boiling or decomposition of the test item could be observed up to 400 °C	Acceptable	Y	Gao, J. (2015)
B.2.2. VAPOUR PRESSURE, VOLATILITY						
Vapour pressure **B.2.2/01**	EEC A.4 OECD 104	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	Experimental value of vapour pressure could not be obtained; the values of vapour pressure were estimated according to OECD Guideline 104. at 20 °C: 1.90 x 10^{-15} Pa at 25 °C: 8.67 x 10^{-15} Pa	Acceptable Effusion method: isothermal thermogravimetry was chosen as a method for the determination of the Vapour pressure (Range 10^{-10} - 1 Pa). However no linear correlation could be obtained in the test. Therefore the calculation method was used as outlined in OECD 104. The boiling point was estimated using the Stein and Brown's Group Contribution Method (Handbook of Property Estimation Methods for Chemicals) to be 560 °C.	Y	Gao, J. (2015)
Volatility (Henry's Law constant) **B.2.2/02**	Calculation	-	2.4 x 10^{-13} Pa.m³.mol^{-1} (Vapor pressure / water solubility) [at 20 °C]	Acceptable	-	-

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)						
Physical state and colour **B.2.3/01**	-	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	Pale white solid	Acceptable	N	Gao, J. (2015)
	-	24-Epibrassinolide TGAI Batch No. 002-20140512 92.3% purity	Oyster white solid	Acceptable	N	Gao, J. (2015)
B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY						
Ultraviolet/visible (UV/VIS) **B.2.4/01**	OECD 101	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	UV/VIS (neutral) [water/Acetonitrile 4:1 v/v] pH 5.57 Wavelength [nm] / Molar extinction coefficient [L/mol x cm] 205 / 183 215 / 91 UV/VIS (acidic) [1M HCl/water/Acetontrile 1:8:2 v/v/v] pH 0.6 Wavelength [nm] / Molar extinction coefficient [L/mol x cm] 200 / 245 UV/VIS (alkaline) [1M NaOH/water/Acetontrile 1:8:2 v/v/v] pH 13.4 Wavelength [nm] / Molar extinction coefficient [L/mol x cm] 219 / 67	Acceptable	Y	Gao, J. (2015)

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results		Comments (Acceptable / Non acceptable)	GLP	Reference
Infrared (IR) **B.2.4/02**	-	24-Epibrassinolide Batch No. 24-BYTSNZ-SD-1501 98.3% purity	The spectrum is consistent with the structure of 24-Epibrassinolide		Acceptable	Y	Gao, J. (2015b)
Nuclear magnetic resonance (NMR) **B.2.4/03**	-	24-Epibrassinolide Batch No. 24-BYTSNZ-SD-1501 98.3% purity	^{1}H-NMR The spectra confirmed the structure		Acceptable	Y	Gao, J. (2015b)
Mass spectra (MS) **B.2.4/04**	-	24-Epibrassinolide Batch No. 24-BYTSNZ-SD-1501 98.3% purity	Mass spectrum The spectrum confirmed the structure		Acceptable	Y	Gao, J. (2015b)
B.2.5. SOLUBILITY IN WATER							
Solubility in water **B.2.5/01**	EEC A.6	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	3.8 mg/L at 20 °C (purified water) Investigation of the influence of pH on solubility is not required as test item shows no dissociation in water in the range of pH 1.77 –12.51.		Acceptable	Y	Gao, J. (2015)
B.2.6. SOLUBILITY IN ORGANIC SOLVENTS							
Solubility in organic solvents **B.2.6/01**	EEC A.6 OECD 105	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	solvent	solubility [mg/L] at 20 °C	Acceptable	Y	Gao, J. (2015)
			heptane	< 3.1			
			toluene	19.1			
			dichloromethane	5953			
			methanol	28715			
			acetone	17988			
			ethyl acetate	5514			

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER						
Partition coefficient n-octanol/water B.2.7/01	EEC A.8 OECD 117	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	log P_{OW} = 2.0 Investigation of the influence of acidic or alkaline pH levels is not required as test item shows no dissociation in water in the range of pH 1.77 –12.51.	Acceptable	Y	Gao, J. (2015)
B.2.8. DISSOCIATION IN WATER						
Dissociation constant B.2.8/01	OECD 112	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	The pKa test was carried out at 29 °C. No acid or base properties were found in the range pH 1.77 –12.51.	Acceptable	Y	Gao, J. (2015)
B.2.9. FLAMMABILITY AND SHELF-HEATING						
Flammability B.2.9/01	EC A.10	24-Epibrassinolide TGAI Batch No. 002-20140512 92.3% purity	24-Epibrassinolide is not ignitable and can thus be considered as not flammable.	Acceptable	Y	Gao, J. (2015)
Self-heating B.2.9/02	EC A.16		No test according to guideline EC A.16 was performed. This test consists of heating the sample to the melting point at 0.5° per minute. A similar test was done to determine the melting point (quick heat to 250°C and then 1°C per minute) see B 2.1/01. A similar test was done for explosive properties where a TGA/DSC was performed with 15 ° per minute up to 500°C. No exothermic peak was found.	Acceptable The TGA/DSC show no sign that the substance is self-heating	Y	Gao, J. (2015)
B.2.10. FLASH POINT						
Flash point B.2.10/01			Not applicable. The active substance is a solid; its melting point is > 40 °C	Acceptable		
B.2.11. EXPLOSIVE PROPERTIES						
Explosive properties B.2.11/01	statement		Considering the structural formula and the negative oxygen balance 24-Epibrassinolide is considered non-explosive	Acceptable	N	Feyrer, A.; Goerg, J. (2017)

B.2.12. SURFACE TENSION						
Surface tension **B.2.12/01**	EC A.5. OECD 115	24-Epibrassinolide Batch No. 002-20150323 97.2% purity	The surface tension of a 90% saturated solution of 24-Epibrassinolide at 20°C is 68 mN m^{-1}. not surface active.	Acceptable	Y	Gao, J. (2015)
B.2.13. OXIDISING PROPERTIES						
Oxidizing properties **B.2.13/01**	statement		Considering the structural formula and the negative oxygen balance 24-Epibrassinolide is considered non-oxidizing	Acceptable	N	Feyrer, A.; Goerg, J. (2017)
B.2.14. OTHER STUDIES						
			None			

24-Epibrassinolide as technical grade substance is an oyster white solid, while the pure active substance is a pale white solid. The melting point was determined to be 254.6–258.2 °C and no boiling or decomposition of the test item could be observed up to 400 °C. Values for the vapour pressure have been estimated to amount to 1.90 x 10^{-15} Pa at 20 °C and 4.6 x 10^{-8} Pa at 25°C, respectively. 24-Epibrassinolide is characterised by a rather low solubility in water (3.8 mg/l, pH 4.8) and in n-heptane (<3.08 mg/l) at 20 °C. Higher solubilities are obtained in ethyl acetate (5514 mg/l), in dichloromethane (5953 mg/l), in acetone (17988 mg/l), and in methanol (28715 mg/l) at 20 °C. The partition coefficient (n-octanol/water) was found to be 2.0. No dissociation in water has been observed in the range between pH 1.77–12.51. The surface tension amounts to 68 mN/m at 20.0 °C.

24-Epibrassinolide is not flammable, explosive or has any oxidising properties and therefore does not require classification for physico-chemical hazards.

B.2.15. REFERENCES RELIED ON

Data Point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evaluation
KCA 2.1/01 KCA 2.1/02 KCA 2.1/03 KCA 2.2/01 KCA 2.2/02 KCA 2.3/01 KCA 2.4/01 KCA 2.5/01 KCA 2.6/01 KCA 2.7/01 KCA 2.8/01 KCA 2.9/01 KCA 2.9/02 KCA 2.12/01	Gao, J.	2015	CHEMICAL AND PHYSICAL CHARACTERIZATION OF 24-EPIBRASSINOLIDE TGAI Report No.: NC-2015-033 (119-001) Nutrichem Laboratory Co., Ltd., Beijing, China GLP, unpublished	N	Y	New study necessary for the approval of 24-Epibrassinolide	Suntton GmbH	N
KCA 2.4/02 KCA 2.4/03 KCA 2.4/04	Gao, J.	2015b	PRELIMINARY ANALYSIS AND ENFORCEMENT ANALYTICAL METHOD OF 24-EPIBRASSINOLIDE TGAI Report No.: NC-2015-032 (172-001) Nutrichem Laboratory Co., Ltd., Beijing, China GLP, unpublished	N	Y	New study necessary for the approval of 24-Epibrassinolide	Suntton GmbH	N
KCA 2.11/01 KCA 2.13/01	Feyrer, A. Goerg, J.	2017	STATEMENT RELATED TO THE EXPLOSIVE AND OXIDISING PROPERTIES OF 24-EPIBRASSINOLIDE - ACTIVE SUBSTANCE: 24-EPIBRASSINOLIDE Report No.: PP309-00002-17/01 (181-001) Scientific Consulting Company, Bad Kreuznach, Germany Not GLP, unpublished	N	Y	New study necessary for the approval of 24-Epibrassinolide	Suntton GmbH	N