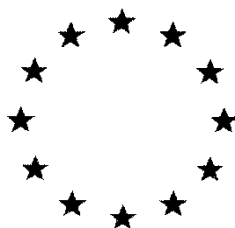


# *European Commission*



**Draft (Renewal) Assessment Report prepared according to the Commission  
Regulation (EU) N° 1107/2009**

**TRITICONAZOLE**

**Volume 3 – B.2 (AS)**

Rapporteur Member State: Austria  
Co-Rapporteur Member State: United Kingdom

## Version History

When	What
2003/ September	Initial DAR, first version
2004/ September	Addendum 1
2005/January	Addendum rev. 2
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## **B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE**

Throughout this document the original DAR, is referred to as the DAR 2003 and this evaluation, is referred to as the RAR (Renewal assessment report). Studies that were evaluated in the DAR 2003 have not been re-evaluated and the results are presented in this report in **grey typeface**. New information (e.g. historical control data, additional experimental details) or new interpretation of the data has been taken into account or changes compared to the original DAR 2003 are written in **black typeface**.

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
<b>B.2.1. MELTING POINT AND BOILING POINT</b>						
<b>Melting, freezing or solidification point</b> B.2.1/01	EC A.1 Differential scanning calorimetry	998.5 g/kg Pure active substance	First crystalline form: 137 °C Second crystalline form: 141 °C	EU agreed endpoint DAR 2003	Y	Cousin et al., 1993
<b>Boiling point</b> B.2.1/02	EC A.2 Differential scanning calorimetry	998.5 g/kg Pure active substance	Not measurable, see B.2.1/03	EU agreed endpoint DAR 2003	Y	Cousin et al., 1993
<b>Decomposition / Sublimation temperature</b> B.2.1/03	EC A.1 Differential scanning calorimetry	998.5 g/kg Pure active substance	After the test substance melted, the product was found to start slightly decomposing. This decomposition process became significant at temperatures above 180 °C.	EU agreed endpoint DAR 2003	Y	Cousin et al., 1993
<b>B.2.2. VAPOUR PRESSURE, VOLATILITY</b>						
<b>Vapour pressure</b> B.2.2/01	EC A.4 OECD 104 vapour pressure balance	986 g/kg Pure active substance	9 x 10 <sup>-8</sup> Pa at 25 °C	<b>Acceptable</b> The study was conducted to comply with the requirements of Regulation 283/2013.	Y	Cowlyn N., 2014a 2014/1001862
<b>Volatility (Henry's Law constant)</b> B.2.2/02	Calculation	N/A	K <sub>H</sub> = 1.2 x 10 <sup>-6</sup> Pa m <sup>3</sup> /mole at 20 °C <u>Parameters for calculation:</u> vp : 3.6 x 10 <sup>-8</sup> Pa at 20 °C ws : 9.3 mg/L at 20 °C	<b>Acceptable</b>	N	Daum A., 2015 2015/1256390

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	Visual assessment	998.5 g/kg	Powder	EU agreed endpoint DAR 2003	Y	Chabassol et al., 1992
		998.5 g/kg	White			
		957 & 959 g/kg	Powder with or without agglutinated mass			
		957 & 959 g/kg	White			
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	993 g/kg	Neutral medium (MeOH/Water 100:10)  Wavelength (nm) $\epsilon$ (L x mol <sup>-1</sup> x cm <sup>-1</sup> ) 212    23879 263    25731  No significant modifications were observed between the spectrum obtained in neutral, acidic or basic media.	EU agreed endpoint DAR 2003	Y	Jendrzeczak et al., 1993
	L85-136 (Internal company method)	994 g/kg	<u>UV absorption at 290 nm:</u>  $\epsilon$ (L x mol <sup>-1</sup> x cm <sup>-1</sup> ) in methanol:                                      1555 in water:    1884 in water (acidic conditions):                      1734 in water (basic conditions):                      1869  The absorption between 310 nm - 320 nm is negligible (<< 10 L x mol <sup>-1</sup> x cm <sup>-1</sup> ) in all tested solutions.	Acceptable	Y	Daum A., 2015 2015/1256391
Infrared (IR) B.2.4/02	OECD 101	993 g/kg	Wave number (cm <sup>-1</sup> )    Group assignment 3140    OH stretching (associated)	EU agreed endpoint DAR 2003	Y	Garnier et al., 1992
Nuclear magnetic resonance (NMR) B.2.4/03	OECD 101	993 g/kg	1H NMR Spectrum  $\delta$ (ppm)                                      Multiplicity, J (Hz) 8.11    singlet 7.85    singlet	EU agreed endpoint DAR 2003	Y	Garnier et al., 1992

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			7.23 doublet, 8.5 7.05 doublet, 8.5 5.59 triplet, 2.4 4.36/4.21 doublet, 13.7 3.14 singlet (broad) 2.64 multiplet 1.75 multiplet 1.13 singlet 0.90 singlet			
Mass spectra (MS) B.2.4/04	OECD 101	993 g/kg	m/z 317 Assignment 235 molecular ion M <sup>+</sup> 83 base peak (M-CH <sub>2</sub> Tz) <sup>+</sup> Tz = Triazole (CH <sub>3</sub> Tz) <sup>+</sup>	EU agreed endpoint DAR 2003	Y	Garnier et al., 1992
Spectra for impurities B.2.4/05			Methanol is considered of environmental or toxicological significance for renewal.	As it is a well-known compound no spectra for identification are required		
<b>B.2.5. SOLUBILITY IN WATER</b>						
Solubility in water B.2.5/01	EC Method A.6, OECD 105	993 g/kg	Dist. Water (pH 7.3 – 8.7; 20) 9.3 mg/L 9.3 mg/L at 20 °C	EU agreed endpoint DAR 2003	Y	Chabassol et al., 1991
<b>B.2.6. SOLUBILITY IN ORGANIC SOLVENTS</b>						
Solubility in organic solvents B.2.6/01	US EPA Guidelines D, 63-8  Flask method	959 g/kg	Solvent Solubility at 20°C (g/L) Hexane 0.12 Toluene 12.6 Methanol 18.2 2-Propanol 7.6 1-Octanol 6.2 Dichloromethane 191.0 Acetone 74.5 Ethyl acetate 48.6	EU agreed endpoint DAR 2003	Y	Chabassol et al., 1991

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
<b>B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER</b>						
<b>Partition coefficient n-octanol/water B.2.7/01</b>	EC Method A8 OECD 117	993 g/kg	Log P <sub>ow</sub> = 3.29 ± 0.04 at 20°C The influence of the pH value on the partition coefficient was not investigated. The notifier states that based on the molecular structure no dissociation is expected in aqueous solution.	EU agreed endpoint DAR 2003	Y	Chabassol et al., 1991
	EC Method A8 OECD 117	RPA 404766 993 g/kg	pH 4: Log P <sub>ow</sub> = 1.6 at 25°C pH 7: Log P <sub>ow</sub> = 1.6 at 25°C pH 10: Log P <sub>ow</sub> = 1.5 at 25°C	<b>Acceptable</b> The study is concerning a metabolite and was evaluated for other sections. Therefore it will not be considered as relied on for section 1.	Y	Cowlyn N., 2014b 2014/1001865
	EC Method A8 OECD 117	RPA 407922 995 g/kg	pH 4: Log P <sub>ow</sub> = 1.9 at 25°C pH 7: Log P <sub>ow</sub> = 1.6 at 25°C pH 10: Log P <sub>ow</sub> = 0.04 at 25°C	<b>Acceptable</b> The study is concerning a metabolite and was evaluated for other sections. Therefore it will not be considered as relied on for section 1.	Y	Cowlyn N., 2014c 2014/1001866
	EC Method A8 OECD 117	RPA 406341 918 g/kg	pH 4: Log P <sub>ow</sub> = 2.2 at 25°C pH 7: Log P <sub>ow</sub> = 2.2 at 25°C pH 10: Log P <sub>ow</sub> = 2.1 at 25°C	<b>Acceptable</b> The study is concerning a metabolite and was evaluated for other sections. Therefore it will not be considered as relied on for section 1.	Y	Cowlyn N., 2014d 2014/1001864
	EC Method A8 OECD 117	RPA 406203 999 g/kg	pH 4: Log P <sub>ow</sub> = 3.5 at 25°C pH 7: Log P <sub>ow</sub> = 3.5 at 25°C pH 10: Log P <sub>ow</sub> = 3.5 at 25°C	<b>Acceptable</b> The study is concerning a metabolite and was evaluated for other sections. Therefore it will not be considered as relied on for section 1.	Y	Cowlyn N., 2014e 2014/1001863
<b>B.2.8. DISSOCIATION IN WATER</b>						
<b>Dissociation constant B.2.8/01</b>	OECD 112		No dissociation is expected in aqueous solution. The examination of the chemical structure shows that there is no substituent which could be easily ionised and make the substance ionisable over the range of pH 3-9.	EU agreed endpoint DAR 2003	N	Cousin J., 1994
<b>B.2.9. FLAMABILITY AND SHELF-HEATING</b>						
<b>Flammability B.2.9/01</b>	EC Method A.10	968 g/kg	Not highly flammable	EU agreed endpoint DAR 2003	Y	Mullee, D.M. 1992a
<b>Self heating B.2.9/02</b>	Method 14.3.4 of the UN	971 g/kg	Neither self ignition nor exothermic behaviour were observed when the test substance was maintained at 140	EU agreed endpoint DAR 2003	Y	Vandermarliere, 1992

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	recommendations for transport of dangerous goods		°C for 24 hours.			
<b>B.2.10. FLASH POINT</b>						
Flash point B.2.10/01			Not applicable as the melting point is > 40°C			
<b>B.2.11. EXPLOSIVE PROPERTIES</b>						
Explosive properties B.2.11/01	EC Method A.14	911 g/kg	Not explosive	EU agreed endpoint DAR 2003	Y	Francois, J.M. 2000
<b>B.2.12. SURFACE TENSION</b>						
Surface tension B.2.12/01	EC Method A5 OECD 115	986 g/kg	90% saturated solution: 72.0 mN/m at 20 °C	<b>Acceptable</b> The study was conducted to comply with the requirements of Regulation 283/2013.	Y	Cowlyn N., 2014a 2014/1001862
<b>B.2.13. OXIDISING PROPERTIES</b>						
Oxidizing properties B.2.13/01	EC Method A.17	968 g/kg	The test material has been determined to be non-oxidising	EU agreed endpoint DAR 2003	Y	Mullee D.M., 1992
<b>B.2.14. OTHER STUDIES</b>						
			None			



Triticonazole is a white powder with a melting point of 137 to 141°C. It has a very low vapour pressure and is very slightly volatile. It has low solubility in water 9.3 mg/L at 20°C, whereas higher solubility in organic solvents such as dichloromethane. It does not dissociate in water and has a partition coefficient (log Pow) of 3.3, indicating a potential for bioaccumulation. Triticonazole does not possess explosive or oxidising properties and is neither flammable nor auto-flammable, indicating that it does not present problems during transport or storage. There are no implications for classification.

**B.2.15. REFERENCES RELIED ON**

<b>Data Point</b>	<b>Author(s)</b>	<b>Year</b>	<b>Title Compagny Report No. Source (where different from company) GLP or GEP status Published or not</b>	<b>Vertebrate study Y/N</b>	<b>Data protection claimed Y/N</b>	<b>Justification if data protection is claimed</b>	<b>Owner</b>	<b>Previous evaluation</b>
KCA 2.1	Cousin J.A.	1993a	Stability of RPA 400727 active ingredient above its melting point Rhone-Poulenc - Secteur Agro; Lyon; France R013077 Yes unpublished	N	N	Not applicable	BCS	Yes
KCA 2.1	Cousin J.A.	1993a	Stability of RPA 400727 active ingredient above its melting point Rhone-Poulenc - Secteur Agro; Lyon; France R013077 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.1	Cousin J.A.	1993a	Stability of RPA 400727 active ingredient above its melting point Rhone-Poulenc - Secteur Agro; Lyon; France R013077 Yes unpublished	N	Y	Not applicable	BCS	Yes
no KCA data point	Smeyskal H.	2000a	Triticonazole - AE C632720 00 1B - Relative density Siemens Axiva GmbH & Co. KG; Frankfurt/Main; Germany Fed.Rep. C010910 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.2	Chabassol Y.C., Gomez J.-L.	1992a	RPA 400727 technical grade vapor pressure curve Rhone-Poulenc - Secteur Agro; Lyon; France R013034 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.2	Emeric G.T.	2000a	Triticonazole active ingredient vapor pressure determination - Discussion on the influence of the purity of the test sample Aventis CropScience GmbH; Frankfurt/Main; Germany Fed.Rep. C010434 No, not subject to GLP regulations unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.2	Chabassol Y.	1992a	RPA400727 - Constante de Henry Rhone-Poulenc - Secteur Agro; Lyon; France R013101 No, not subject to GLP regulations unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.2/1	Cowlyn N.	2014 a	Triticonazole - Surface tension and vapour pressure	No	Yes	New data for AIR3 renewal	BASF	No

Data Point	Author(s)	Year	Title Compagny Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection n claimed Y/N	Justification if data protection is claimed	Owner	Previous evaluation
			2014/1001862 Huntingdon Life Sciences Ltd., Eye Suffolk IP23 7PX, United Kingdom yes Unpublished					
KCA 2.2/2	Miles D., Liney P.	2015 a	Triticonazole - Henrys Law Constant 2015/1137136 Exponent International Ltd., Harrogate Yorkshire HG2 8RE, United Kingdom no Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 2.2/3	Daum A.	2016 a	Henrys Law Constant for Triticonazole (BAS 595 F, Reg.No. 4378513) 2015/1256390 BASF SE, Limburgerhof, Germany Fed.Rep. no Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 2.3	Chabert M.S.	1992a	RPA 400727 - Lot EA3010SD7 - Suitability for use as an analytical standard Rhône-Poulenc - Secteur Agro; Lyon; France R013060 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.3	Chabassol Y.C., Gomez J.-L.	1992b	RPA400727 - Technical grade - Physical properties and pH determination Rhône-Poulenc - Secteur Agro; Lyon; France R013042 Yes unpublished	N	Y	Not applicable	BCS	Yes
no KCA data point	Chabassol Y.C., Gomez J.-L.	1992b	RPA400727 - Technical grade - Physical properties and pH determination Rhône-Poulenc - Secteur Agro; Lyon; France R013042 Yes unpublished	N	Y	Not applicable	BCS	Yes
no KCA data point	Chabert M.S.	1992a	RPA 400727 - Lot EA3010SD7 - Suitability for use as an analytical standard Rhône-Poulenc - Secteur Agro; Lyon; France R013060 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.4	Jendrzczak N., Maestracci M.P.	1993a	RPA400727: UV-visible characteristics Rhône-Poulenc - Secteur Agro; Lyon; France R012065 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.4	Garnier C.M.A. et al.	1992a	RPA400727 - NMR, IR and MS spectra	N	Y	Not applicable	BCS	Yes

Data Point	Author(s)	Year	Title Compagny 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
			Rhone-Poulenc - Secteur Agro; Lyon; France R012059 Yes unpublished					
KCA 2.4/1	Daum A.	2015 a	UV/VIS Spectrum of Triticonazole (Reg.No. 4378513, BAS 595 F) PAI 2015/1256391 BASF SE, Limburgerhof, Germany Fed.Rep. yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 2.5	Chabassol Y.C., Gomez J.L.	1991a	RPA 400727 - Water solubility Rhone-Poulenc - Secteur Agro; Lyon; France R013020 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.6	Chabassol Y.C., Gomez J.-L.	1991a	RPA 400727 technical grade - Solubility in organic solvents Rhone-Poulenc - Secteur Agro; Lyon; France R012057 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.7	Chabassol Y.C., Gomez J.L.	1991b	RPA 400727 - Octanol/water partition coefficient at 20° C Rhone-Poulenc - Secteur Agro; Lyon; France R013026 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.8	Corgier M.M.C., Robin J.M.	1991a	14C-RPA 400727 - Hydrolysis at 25°C Rhone-Poulenc - Secteur Agro; Lyon; France R013023 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.8	Corgier M.M., Robin J.M.	1992a	14C-RPA 400727: Aqueous photolysis Rhone-Poulenc - Secteur Agro; Lyon; France R013068 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.8	Gorgier M.M., Turier G.P.	1995a	Triticonazole - Quantum yield and environmental half-life in water Rhone-Poulenc - Secteur Agro; Lyon; France R012072 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.8	Cousin J.	1994a	RPA 400727 active ingredient - Assessment for ionisation constant determination Rhone-Poulenc - Secteur Agro; Lyon; France	N	Y	Not applicable	BCS	Yes

Data Point	Author(s)	Year	Title Compagny Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection n claimed Y/N	Justification if data protection is claimed	Owner	Previous evaluation
			R013118 No, not subject to GLP regulations unpublished					
no KCA data point	Voelkel W.	1999a	Estimation of the degradation of Triticonazole by photo-oxidation in air RCC Ltd.; Itingen; Switzerland R012052 No, not subject to GLP regulations unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.9	Mullee D.M.	1992a	RPA 400727 (Lot No: DA 646) - Determination of flammability (solids) Safepharm Laboratories Ltd.; Derby Derbyshire DE1 2BT; United Kingdom R013070 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.9	Vandermarliere P.	1992a	RPA 400727 - Minimum ignition energy, lower explosive limit (dust cloud) and auto ignition (layer) Rhône-Poulenc Industrialisation; Decines Charpieu; France R013095 No unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.11	Francois J.M.	2000a	Triticonazole - Determination of the explosion properties and ability for self heating Rhoditech; Decines Charpieu; France R012101 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.12	Mullee D.M.	1992b	RPA 400727 (Lot No: DA 646) - Determination of surface tension Safepharm Laboratories Ltd.; Derby Derbyshire DE1 2BT; United Kingdom R013072 Yes unpublished	N	Y	Not applicable	BCS	Yes
KCA 2.12/1	Cowlyn N.	2014 a	Triticonazole - Surface tension and vapour pressure 2014/1001862 Huntingdon Life Sciences Ltd., Eye Suffolk IP23 7PX, United Kingdom yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 2.13	Mullee D.M.	1992c	RPA 400727 (Lot No. DA 646) - Determination of oxidising properties Safepharm Laboratories Ltd.; Derby Derbyshire DE1 2BT; United Kingdom	N	Y	Not applicable	BCS	Yes

<b>Data Point</b>	<b>Author(s)</b>	<b>Year</b>	<b>Title Compagny Report No. Source (where different from company) GLP or GEP status Published or not</b>	<b>Vertebrate study Y/N</b>	<b>Data protection n claimed Y/N</b>	<b>Justification if data protection is claimed</b>	<b>Owner</b>	<b>Previous evaluation</b>
			R013071 Yes unpublished					