

# **Renewal Assessment Report**

## **Dimethenamid-P**

**Volume 3 – B.2 Physical and chemical properties**

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**Co-Rapporteur Member State: Bulgaria**

## Version history

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## B.2 Physical and chemical properties of the active substance

Study	Method	Purity [%]	Results	Conclusion/ Comment	GLP	Reference
<b>B.2.1 Melting point and boiling point (CA 2.1)</b>						
Melting, freezing or solidification point	OECD 102 EC A 1 (DSC)	99.4	Solidification point below –50 °C	acceptable (DAR)	Y	Kröhl (1999) (CHE1999-1052)
	OECD 102 (DSC)	94.0	no thermal effect between -50 °C and 101 °C	additional information as technical active substance was used	Y	Daum (2004) (BVL no. 2630035)
Boiling point	OECD 103 EC A 2	99.4	No boiling point detected until 280 °C	acceptable (DAR)	Y	Kröhl (1999) (CHE1999-1052)
	US-EPA no. 63-3 EC A 2 (dynamic method)	94.6	122.6 °C at 9.3 Pa	supplementary information, acceptable (DAR)	Y	Chen (1999) (CHE1999-1053)
	OECD 103 (Siwoloboff)	94.0	no boiling point up to 210 °C	additional information as technical active substance was used	Y	Daum (2004) (BVL no. 2630035)
Decomposition / Sublimation temperature	OECD 102 (DSC)	94.0	101 °C (slow decomposition)	additional information as technical active substance was used	Y	Daum (2004) (BVL no. 2630035)

Study	Method	Purity [%]	Results	Conclusion/Comment	GLP	Reference
<b>B.2.2 Vapour pressure, volatility (CA 2.2)</b>						
Vapour pressure	US-EPA, no. 63-9 EC A 4 (gas saturation method)	98.6	$3.47 \times 10^{-3} \pm 1.29 \times 10^{-3}$ Pa (20 °C) $2.51 \times 10^{-3} \pm 0.39 \times 10^{-3}$ Pa (25 °C)	acceptable (DAR)  The HPLC-UV method used for analysis is adequately validated.	Y	Chen and Laster (1996) (LUF1999-145)
Volatility (Henry's Law constant)	Calculation		$4.8 \times 10^{-4}$ Pa m <sup>3</sup> mol <sup>-1</sup> (25 °C)	acceptable (DAR)	Y	Hsieh (1999) (LUF1999-146)
<b>B.2.3 Appearance (physical state, colour) (CA 2.3)</b>						
Appearance (physical state, colour)	Visual assessment	99.4	colour: clear yellow brown (at room temperature) physical state: liquid odour: faint aromatic	acceptable (DAR)	Y	Kröhl (1999) (CHE1999-1052)
		94.6	colour: dark brown (at room temperature) physical state: liquid	acceptable (DAR)	Y	Chen (1997) (CHE1999-1055)
			odour: strong unpleasant musty	acceptable (DAR)	Y	Jones (1997) (CHE1999-1056)
	Visual assessment	94.0	colour: slightly brown (at diffused daylight) physical state: liquid odour: faint intrinsic odour condition: clear liquid	acceptable	Y	Daum (2004) (BVL no. 2630036)
<b>B.2.4 Spectra (UV/VIS, IR, NMR, MS), molar extinction at relevant wavelengths, optical purity (CA 2.4)</b>						
Spectra (UV/VIS, IR, NMR, MS), molar extinction at relevant wavelengths, optical purity	UV-VIS US-EPA OPPTS 830.7050	99.4	$\lambda_{\max}$ [nm] $\epsilon$ [L mol <sup>-1</sup> cm <sup>-1</sup> ] 236                      7560	acceptable (DAR)	Y	Bauer and Cristy (1998) (CHE1999-1057)
	UV, IR,	96.5	Spectra are consistent with given structure of	acceptable (DAR)	Y	Kirstgen (1999)

Study	Method	Purity [%]	Results	Conclusion/ Comment	GLP	Reference
	<sup>1</sup> H-NMR, MS		dimethenamid-P.			(CHE1999-1058) (CHE1999-1059)
Spectra for impurities	UV-VIS, IR, NMR, MS		Spectra of Keto-Enol and TCE are announced to be finished by end of March 2016.	Spectra of the relevant impurities are missing.		
<b>B.2.5 Solubility in water (CA 2.5)</b>						
Solubility in water	EC A 6 (column elution method)	98.6	1499 ± 17 mg/L at 25 °C (pH 6.16 ± 0.28)  There is no dissociation in water therefore pH dependence on solubility is not applicable	acceptable (DAR)  The HPLC-UV method used for analysis is adequately validated.	Y	Laster (1996) (CHE1999-1060)
<b>B.2.6 Solubility in organic solvents (CA 2.6)</b>						
Solubility in organic solvents	US-EPA, no. 63-8	93.1	Soluble in all proportions in tetrahydrofuran, isopropyl alcohol, acetone, acetonitrile, dimethyl sulfoxide, dichloromethane, toluene and n-octanol at 25 °C. The solubility in hexane at 25 °C is 20.8 g per 100 mL of saturated solution.	acceptable (DAR)  The HPLC-UV method used for the determination of hexane is adequately validated.	Y	Liu (1997) (CHE1999-1061)
	CIPAC MT181	96.4	<i>n</i> -Heptane 310 - 330 <i>n</i> -Hexane 310 - 330 Toluene > 1000 Dichloromethane > 1000 Methanol > 1000 Acetone > 1000 Ethyl acetate > 1000 Acetonitrile > 1000  all values in g/L at 20 °C	acceptable	Y	Class (2006) (BVL no. 2630038)

Study	Method	Purity [%]	Results	Conclusion/ Comment	GLP	Reference
<b>B.2.7 Partition coefficient n-octanol/water (CA 2.7)</b>						
Partition coefficient n-octanol/water	EC A 8 (shake flask method) (liquid scintillation counting)	94.45 96.0 ( <sup>14</sup> C-labelled)	log P <sub>o/w</sub> = 1.89 (25 °C) Effect of pH was not investigated since there is no dissociation in water.	acceptable (DAR)	Y	Lam (1998) (CHE1999-1062)
Partition coefficient n-octanol/water of metabolites				Studies for the determination of the partition coefficient of all metabolites of the residue definition for risk assessment are required.		
<b>B.2.8 Dissociation in water (CA 2.8)</b>						
Dissociation constant	US-EPA No. 63-10 OECD 112	98.0 (racemic dimethenamid)	UV spectrophotometric investigation gave no indication of dissociation of dimethenamid taking place between pH of 1 and 11 at 25 °C.	acceptable (DAR)	Y	Rozek (1988) (WAS1999-167)
<b>B.2.9 Flammability and self-heating (CA 2.9)</b>						
Flammability			Not required. TAS is a liquid and does not evolve highly flammable gases.	acceptable (DAR)		
Self-heating	EC A 15	97.9 (racemic dimethenamid)	The auto-ignition temperature was determined to be 395 °C.	acceptable (DAR)	Y	van Helvoirt (1994) (CHE1999-1064)
<b>B.2.10 Flash point (CA 2.10)</b>						
Flash point	EC A 9	93.5	The flash point of the TAS is 79 °C.	acceptable (DAR)	Y	Widlak (1997) (CHE1999-1065)

Study	Method	Purity [%]	Results	Conclusion/ Comment	GLP	Reference
<b>B.2.11 Explosive properties (CA 2.11)</b>						
Explosive properties	US-EPA No. 63-16 (partially ful-fils EC A 14)	96.73 (racemic dimethenamid)	The result of the explosive impact test indicated that technical dimethenamid is not an impact explosive sensitive compound.	acceptable (DAR)	Y	Srnak (1991) (CHE1999-1066)
	OECD 102 (DSC/TG)	96.4	Technical DMTA-P is thermally stable, as the DSC/TG-curve does not show any thermal effect at normal pressure between -5 °C and 170 °C which could be related to solidification, melting or boiling, respectively. Above approx. 170 °C two endothermic peaks appear accompanied by a two-step mass loss of more than 90 % in total. These effects are assigned to decomposition of the test item and vaporisation of the cracked products. Further tests for explosive properties were omitted, as no exothermic effects were observed.	not acceptable The test is not in compliance with method EC 14.	Y	Kröhl (2006) (BVL no. 2630039)
	OECD 102 (DSC)	94.0	For the TGAI, no thermal effect was observed at normal pressure between -50 °C and 400 °C which could be related to solidification, melting or boiling respectively. Above 101 °C a weak broad endothermic effect shows up in the DSC curve accompanied by loss of 80 % of the sample weight. The phenomenon is assigned to vaporisation of the cracked products.	not acceptable The test is not in compliance with method EC 14.	Y	Daum (2004) (BVL no. 2630040)
<b>B.2.12 Surface tension (CA 2.12)</b>						
Surface tension	EC A 5 (plate method)	99.4	52.0 mN/m (0.1 % (w/w), 20 °C) 50.7 mN/m (0.5 % (w/w), 20 °C)	acceptable (DAR)	Y	Kröhl (1999) (CHE1999-1052)
<b>B.2.13 Oxidising properties (CA 2.13)</b>						
Oxidising properties	US-EPA	93.0	Study of reactions with oxidising and reducing	The study which	Y	Jones (1998)



Study	Method	Purity [%]	Results	Conclusion/ Comment	GLP	Reference
	OPPTS 830.6314		agents indicated that dimethenamid exhibits mild reaction with potassium permanganate. Contact with strong oxidising agents should be avoided.	Was accepted in the DAR, but does not address the data requirement of oxidising properties (support of fire). However, additional data are not necessary since the oxygen and chlorine in the compound are only chemically bonded to carbon.		(CHE1999-1067)
<b>B.2.14 Other studies</b>						
Other studies	–	–	–	–	–	–

## B.2.15 References relied on

Data Point  EU as of 2014	Author(s)	Year	Date	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	Previously submitted Y/N  If yes, old data point
KCA 2.1	Kroehl T.	1999	09.02.1999	Physical properties of dime-thenamid-p (PAI) BASF Aktiengesellschaft, Limburgerhof, Germany BASF RegDoc.# 99/10167 GLP, unpublished CHE1999-1052	N	N	Not applicable	BASF	Y relevant IIA. 2.1.2 [2.1/01]
KCA 2.1	Chen H.	1999	19.03.1997	Boiling point of SAN 1289H SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.# 97/5194 GLP, unpublished CHE1999-1053	N	N	Not applicable	BASF	Y relevant IIA. 2.1.2 [2.1/02]
KCA 2.1/1	Daum A.	2004	14.04.2004	Determination of the melting point/boiling point and the appearance of Dimethenamid-P (BAS 656 H, Reg.No. 363 851) PAI 2004/1010746 BASF AG Agrarzentrum Limburgerhof, Limburgerhof, Germany Fed.Rep. GLP, unpublished BVL no. 2630035	N	Y	New data for AIR3 renewal	BASF	N II A 2.1
KCA 2.2	Chen H., Laster W.	1996	18.09.1996	Vapor pressure of SAN 1289H SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#96/5418 GLP, unpublished LUF1999-145	N	N	Not applicable	BASF	Y relevant IIA. 2.3.1 [2.3/01]
KCA 2.2	Hsieh T.	1999	12.01.1999	Henry's law constant of dime-thenamid-p BASF Corp, ARC, RTP, NC USA BASF RegDoc.# 1999/5002 Not GLP, unpublished LUF1999-146	N	N	Not applicable	BASF	Y relevant IIA. 2.3.2 [2.3/02]
KCA 2.3	Chen H.	1997	19.03.1997	Physical state of SAN 1289H SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#97/5198 GLP, unpublished CHE1999-1055	N	N	Not applicable	BASF	Y Not relevant IIA. 2.4.1 [2.4/01]
KCA 2.3	Kroehl T.	1999	09.02.1999	Physical properties of dime-thenamid-p (PAI) BASF Aktiengesellschaft, Limburgerhof, Germany BASF RegDoc.# 99/10167 GLP, unpublished CHE1999-1052	N	N	Not applicable	BASF	Y relevant IIA. 2.4.1 [2.1/01]
KCA 2.3	Jones R.	1997	31.03.1997	Determination of odor of Technical SAN 1289H BASF Corp, ARC, RTP, NC USA BASF RegDoc.#97/5186 GLP, unpublished CHE1999-1056	N	N	Not applicable	BASF	Y Not relevant IIA. 2.4.2 [2.4/02]

Data Point EU as of 2014	Author(s)	Year	Date	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	Previously submitted Y/N If yes, old data point
KCA 2.3/1	Daum A.	2004	14.04.2004	Determination of the melting point/boiling point and the appearance of Dimethenamid-P (BAS 656 H, Reg.No. 363 851) PAI 2004/1010746 BASF AG Agrarzentrum Limburgerhof, Limburgerhof, Germany Fed.Rep. GLP, unpublished BVL no. 2630036	N	Y	New data for AIR3 renewal	BASF	N II A 2.3
KCA 2.4	Bauer M.R., Cristy T	1998	03.06.1998	Ultraviolet-visible (UV/VIS) spectrum of Dimethenamid-p Battelle Laboratories, 505 King Avenue, Columbus, Ohio Laboratories, USA BASF RegDoc.#98/5123 GLP, unpublished CHE1999-1057	N	N	Not applicable	BASF	Y relevant IIA. 2.5.1 [2.5/01]
KCA 2.4	Kirstgen R.	1999	20.04.1999	Charakterisierung der Prüfsubstanz Reg.-Nr. 363 851 (01311-220) BASF Aktiengesellschaft, Limburgerhof, Germany BASF RegDoc.#PCP 05006 (German Original) GLP, unpublished CHE1999-1058	N	N	Not applicable	BASF	Y relevant IIA. 2.5.1 [2.5/02]
KCA 2.4	Kirstgen R.	1999	20.04.1999	Characterisation of reference compound Reg.-Nr. 363 851 (01311-220) BASF Aktiengesellschaft, Limburgerhof, Germany BASF RegDoc.#99/10449 (English translation of PCP 05006) GLP, unpublished CHE1999-1059	N	N	Not applicable	BASF	Y relevant IIA. 2.5.1 [2.5/03]
KCA 2.5	Laster W.	1996	10.05.2019	Solubility of SAN 1289H in water SANDOZ Agro, Inc., Des Plaines, Illinois 60018 96/5411 GLP, unpublished CHE1999-1060	N	N	Not applicable	BASF	Y relevant IIA. 2.6 [2.6/01]
KCA 2.6	Liu J.	1997	25.03.1997	Solubility of Technical SAN 1289H in solvent SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#97/5196 GLP, unpublished CHE1999-1061	N	N	Not applicable	BASF	Y Not relevant IIA. 2.7 [2.7/01]
KCA 2.6/1	Class T.	2006	02.10.2006	Dimethenamid-P (BAS 656 H, Reg.No. 363 851): Determination of solubility in organic solvents 2006/1032688 PTREL Europe GmbH, Ulm, Germany Fed.Rep. GLP, unpublished BVL no. 2630038	N	N	Not applicable	BASF	Y Not relevant IIA. 2.7
KCA 2.7	Lam W.W.	1998	12.05.1998	Determination of the n-octanol/water partition coefficient of Dimethenamid-p BASF Corp, ARC, RTP, NC USA BASF RegDoc.#98/5071 GLP, unpublished CHE1999-1062	N	N	Not applicable	BASF	Y relevant IIA. 2.8 [2.8/01]

<b>Data Point</b> <b>EU as of 2014</b>	<b>Author(s)</b>	<b>Year</b>	<b>Date</b>	<b>Title</b> <b>Company Report No.</b> <b>Source (where different from company)</b> <b>GLP or GEP status</b> <b>Published or not</b>	<b>Vertebrate study</b> <b>Y/N</b>	<b>Data Protection Claimed</b> <b>Y/N</b>	<b>Justification if data protection is claimed</b>	<b>Owner</b>	<b>Previously submitted Y/N</b>  <b>If yes, old data point</b>
KCA 2.8	Rozek A.	1988	25.07.1988	Determination of the dissociation constant of SAN 582H SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#88/11352 GLP, unpublished WAS1999-167	N	N	Not applicable	BASF	Y relevant IIA. 2.9.4 [2.9/04]
KCA 2.9	van Helvoirt J.	1994	20.10.1994	Determination of the auto-ignition temperature (liquids) of dimethenamid technical Novartis Agro c/o Clariant Huningue S.A., Huningue Cedex BASF RegDoc.# 94/11877 GLP, unpublished CHE1999-1064	N	N	Not applicable	BASF	Y relevant IIA. 2.11.2 [2.11/01]
KCA 2.10	Widlak A.	1997	19.03.1997	Flash point of SAN 1289H SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#97/5177 GLP, unpublished CHE1999-1065	N	N	Not applicable	BASF	Y relevant IIA. 2.12 [2.12/01]
KCA 2.11	Srnak Z.	1991	26.09.1991	Explodability of SAN 582H, Technical SANDOZ Agro, Inc., Des Plaines, Illinois 60018 BASF RegDoc.#91/11850 GLP, unpublished CHE1999-1066	N	N	Not applicable	BASF	Y Not relevant IIA. 2.13 [2.13/01]
KCA 2.11/1	Kroehl T.	2006	05.10.2006	Thermal stability of Dimethenamid-P (BAS 656 H, Reg.No. 363 851) 2006/1032689 BASF AG Agrarzentrum Limburgerhof, Limburgerhof, Germany Fed.Rep. GLP, unpublished BVL no. 2630039	N	Y	New data for AIR3 renewal	BASF	N IIA. 2.13
KCA 2.11/2	Daum A.	2004	14.04.2004	Determination of the melting point/boiling point and the appearance of Dimethenamid-P (BAS 656 H, Reg.No. 363 851) PAI 2004/1010746 BASF AG Agrarzentrum Limburgerhof, Limburgerhof, Germany Fed.Rep. GLP, unpublished BVL no. 2630040	N	Y	New data for AIR3 renewal	BASF	N IIA. 2.13
KCA 2.12	Kroehl T.	1999	09.02.1999	Physical properties of dimethenamid-p (PAI) BASF Aktiengesellschaft, Limburgerhof, Germany BASF RegDoc.# 99/10167 GLP, unpublished CHE1999-1052	N	N	Not applicable	BASF	Y relevant IIA. 2.14 [2.1/01]