

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								
Melting pt. 1	Handbook data	No data	result: -127°C pressure: -	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	X
Melting pt. 2	Handbook data	No data	result: -126.1°C pressure: -	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X
Melting pt. 3	Handbook data	No data	result: -126.2°C pressure: -	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	X
Melting pt. 4	Handbook data	No data	result: -127°C pressure: -	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	X
3.1.2 Boiling point								
Boiling pt. 1	Comparative ebulliometry	99.94%	result: 97.15°C pressure: 1013.25 hPa	Study well documented, meets generally accepted scientific principles	No	2	Ambrose & Sprake (1970)	X
Boiling pt. 2	No data	>=99.9%	result: 97.11°C pressure: 1013.25 hPa	Study well documented, meets generally accepted scientific principles	No data	2	Hiaki et al. (1994)	X
Boiling pt. 3	Handbook data	No data	result: 97.2°C	Peer-reviewed	Not	2	Merck (1996)	X

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Boiling pt. 4	Handbook data	No data	pressure: - result: 97.2°C pressure: 1013 hPa	handbook data Peer-reviewed handbook data	applicable Not applicable	2	CRC (2001)	X
3.1.3 Bulk density/ relative density								
Rel. density 1	Handbook data	No data	0.8053 (d20/4)	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	X
Rel. density 2	Handbook data	No data	0.80361 at 20°C	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	X
Rel. density 3	Handbook data	No data	0.8044 (d20/4)	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	X
Rel. density 4	Handbook data	No data	0.8016 (d25/4)	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	X
Rel. density 5	Handbook data	No data	0.79960 at 25°C	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	X
Specific density 6	Handbook data	No data	0.7997 g/cm ³ at 25°C	Peer-reviewed handbook data	Not applicable		CRC (2001)	X
Specific density 7	Oscillating-tube densiometer	1-propanol purified by fractionally distillation (not further specified)	0.799448 g/cm ³ at 25°C	Study well documented, meets generally accepted scientific principles	No data	2	Sakurai & Nakagawa (1984)	X
Specific density 8	No data	≥ 99.9%	0.79965 g/cm ³ at 25°C	Study well documented, meets	No data	2	Hiaki et al. (1994)	X

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				generally accepted scientific principles				
3.2 Vapour pressure (IIA3.2)								
Vapour pressure 1	Handbook data	No data	temperature: 25°C result: 27.98 hPa	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	X
Vapour pressure 2	Handbook data	No data	temperature: 25°C result: 27.6 hPa	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X
Vapour pressure 3	Calculated via Antoine equation	>=99.9%	temperature: 25°C result: 27.26 hPa	generally accepted determination method	No data	2	Hiaki et al. (1994)	X
Vapour pressure 4	Calculated via Antoine equation	No data	temperature: 25°C result: 27.615 hPa	generally accepted determination method	No data	2	Boublik et al. (1984)	X
3.2.1 Henry's Law Constant (Pt. I-A3.2)								
Henry's Law Constant 1	GC	No data	measured: result: 0.751 Pa • m ³ /mol at 25 °C	Study well documented, meets generally accepted scientific principles	No data	2	Snider & Dawson (1985), ITEM (2008)	X
Henry's Law Constant 2	Thermodynamic method in combination with GC or HPLC analysis	Pure (not further specified)	measured: result: 0.372 Pa • m ³ /mol at 25 °C	Study described in sufficient detail	No data	2	Altschuh et al. (1999), ITEM (2008)	X

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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
Henry's Law Constant 3	Calculation (HENRYWIN v3.10)	-	calculated: result: 0.76 Pa • m ³ /mol (bond method) 0.70 Pa • m ³ /mol (group method) at 25 °C each	Generally accepted calculation method	Not applicable	2	EPI-Suite (2005), ITEM (2008)	X
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Handbook data	-	liquid	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	X
3.3.2 Colour	Handbook data	-	clear	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	X
3.3.3 Odour	Handbook data	-	Alcoholic and slightly stupefying	Peer-reviewed handbook data	Not applicable	2	Merck (1996), Sax (1984)	X
3.4 Absorption spectra (IIA3.4)								
UV/VIS	Handbook data	no data	For propan-1-ol as a solvent in UV/VIS spectrophotometry a cut-off point of 210 nm is given. Therefore, no absorption between 290 nm and 750 nm is expected.	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X

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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
IR	UV-Vis	99.83%	Spectrum is consistent with the proposed structure. No absorption maximum >210 nm	Internal report of applicant	N	2	Lysoform (2007)	X
	Carry 50 , single beam, 190 – 800 nm	99.93%	Spectrum is consistent with the proposed structure. No absorption maximum >210 nm	Internal report of manufacturer to applicant	N	2	BASF (2007)	X
	Liquid film	no data	3333, 2963, 2938, 2878, 1656, 1651, 1456, 1383, 1293, 1236, 1100, 1069, 1066, 1017, 969, 905, 888, 858, 755, 479 cm ⁻¹	Compilation of data	Not applicable	2	SDBS (2007)	X
	Not given	99.83%	Spectrum is consistent with the proposed structure compared with reference spectrum	Internal report of manufacturer to applicant	N	2	SASOL (2007)	X
NMR	Liquid film	99.92%	Spectrum is consistent with the proposed structure compared with reference spectrum	Internal report of manufacturer to applicant	N	2	BASF (2007)	X
	¹ H-NMR at 89.56 MHz	no data	ppm in CDCl ₃ CH3: 0.94 (t) CH2: 1.57 (s); 3.582 (t) OH: 0.94 (s) ppm in CDCl ₃	Compilation of data	Not applicable	2	SDBS (2007)	X

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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
MS	¹³ C-NMR at 15.09 MHz		CH3: 10.28 CH2: 25.89; 64.25					
	¹ H-NMR at 400 MHz	99.83%	Spectrum is consistent with the proposed structure	Internal report of manufacturer to applicant	N	2	Lysoform (2008)	X
	¹ H-NMR at 400 MHz	99.92%	Spectrum is consistent with the proposed structure	Internal report of manufacturer to applicant	N	2	BASF (2007)	X
	Handbook data	no data	31(100), 27(19), 29(18), 59(11), 42(9), 60(7), 41(7), 28(7), 43(3), 32(3)	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X
	GC/MS	>99.8	Mass spectrum from two manufacturers are consistent with the proposed structure	Internal report of the applicant	N	2	Lysoform (2007)	X
	GC/MS	99.92%	Spectrum is consistent with the proposed structure	Internal report of manufacturer to applicant	N	2	BASF (2007)	X

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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	
3.5 Solubility in water (IIA3.5)	Water solubility 1	Handbook data	No data	result: dissolves indefinitely in water temperature:- pH:-	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	X
	Water solubility 2	Handbook data	No data	result: dissolves indefinitely in water temperature:- pH:-	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	X
3.6 Dissociation constant (-)	-	-	Scientifically unjustified, see Justification for non-submission.	Expert judgement	Not applicable	2		X	
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Handbook data	No data	result: miscible with acetone, alcohol and ether temperature:-	Peer-reviewed handbook data	Not applicable	2	CRC (2001), Merck (1996), Sax (1984)	X	

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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
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIA3.2)	-	-	Scientifically unjustified, see Justification for non-submission.	Expert judgement	Not applicable	2		X
3.9 Partition coefficient n-octanol/water (IIA3.6)								
log P _{OW} 1	GC	No data	result: 0.30 temperature: - pH: (measured)	Generally accepted determination method without detailed documentation	N	2	Dillingham et al. (1973)	X
log P _{OW} 2	Not stated	No data	result: 0.25 temperature: - pH: 7 (measured)	Reliable source	No data	2	Hansch et al. (1995)	X
log P _{OW} 3	Shake-flask method combined with vapor phase chromatography (GC)	No data	result: 0.34 temperature: - pH: (measured)	Study meets generally accepted scientific principles and is described in sufficient details	N	2	Hansch & Anderson (1967)	X

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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
log P _{ow} 4	Calculation (KOWWIN v1.67)	-	result: 0.35 temperature: - pH: - (calculated)	Generally accepted calculation method	-	2	EPI-Suite (2005)	
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	-	-	Scientifically unjustified, see Justification for non- submission.	Expert judgement	-	2		
3.11 Flammability, including auto- flammability and identity of combustion products (IIA3.8)								
Flammability 1	Handbook data	No data	Flammable liquid	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	
Flammability 2	Handbook data	No data	result: 412°C (ignition temperature)	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	
Flammability 3	Handbook data	No data	result: 440°C (ignition temperature)	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	
3.12 Flash-point (IIA3.9)								
Flash-point 1	Handbook data	No data	result: 22°C	Peer-reviewed handbook data	Not applicable	2	Merck (1996)	

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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
Flash point 2	Handbook data	No data	result: 25°C (closed cup)	Acceptable handbook data	Not applicable	2	Riddick et al. (1986)	
Flash point 3	Handbook data	No data	result: 23°C	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	
Flash point 4	Handbook data	No data	result: 15°C (closed cup)	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	
3.13 Surface tension (IIA3.10)								
Surface tension 1	Handbook data	No data	result: 23.32 mN/m temperature: 25°C	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X
Surface tension 2	Prolabo tensiometer, which employs the Wilhelmy plate principle	>99.7%	result: 23.28 mN/m temperature: 25°C	Study well documented, meets generally accepted scientific principles	No data	2	Vazquez et al. (1995)	X
Surface tension 3	Handbook data	Purity: No data 0.1 % (weight % of solute) = 1g/L	result: 67.1 mN/m temperature: 25°C	Peer-reviewed handbook data, result has been regarded valid by national CA in course of EU RAR for 1-propanol (ESR 793/93/EEC)	Not applicable	2	CRC (1992)	X
3.14 Viscosity (-)	Handbook data	No data	result: 1.945 mPa • s temperature: 25°C	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	X

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3.15 Explosive properties (IIA3.11)								
explosive properties 1	Handbook data	No data	Lower explosive limit in air: 2.1% Upper explosive limit in air: 13.5%	Peer-reviewed handbook data	Not applicable	2	Sax (1984)	
explosive properties 2	Handbook data	No data	Lower explosive limit in air: 2.2% Upper explosive limit in air: 13.7%	Peer-reviewed handbook data	Not applicable	2	CRC (2001)	
3.16 Oxidizing properties (IIA3.12)	-	-	Scientifically unjustified, see Justification for non- submission.	Expert judgement	Not applicable	2		
3.17 Reactivity towards container material (IIA3.13)			Scientifically unjustified, see Justification for non- submission.	Expert judgement	Not applicable	2		

Evaluation by Competent Authorities	
<i>Use separate "evaluation boxes" to provide transparency as to the comments and views submitted</i>	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	2016/05/31
General comment	<p>The main references given for the physical chemical properties are handbook data and are referenced to secondary literature. So in the first step it was checked if main information (e.g. substance, purity and method) is stated in the reference. In a second step we have done a weight of evidence assessment. During the assessment we have compared the values of several literature sources.</p> <p>Based on the fact that for all endpoints several references are already stated, we added only further references when these contain more or other information.</p>
Date	2016/05/31
3.1.1 Melting point	<p>All four references given for the melting point are handbook data and are referenced to secondary literature. So in the first step it was checked if main information (e.g. substance, purity and method) is stated in the reference. In a second step we have done a weight of evidence assessment. During the assessment we have compared the values of several literature sources.</p>
Melting pt. 1	
Melting pt. 2	
Melting pt. 3	The following references could be found:
Melting pt. 4	<ul style="list-style-type: none">• GDL Database: : Value = -126.2 deg C, Source: D'Ans-Lax; 4. Auflage (1983)]• HSDB Database Value: -127 deg C Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1348]
	<p>In this case the given values are all about the value of -127 °C, which is stated in the submitted references.</p> <p>Based on the whole information we decided that the given data for the melting point are acceptable.</p>
Conclusion	<p>The Annotations are related to all four melting point datas.</p> <p>The correct quotation for the following field entries are:</p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p>
Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2016/05/31
3.1.2 Boiling point	<p>For the Boiling point three references are handbook data and one reference is a well-documented study.</p>
Boiling pt. 1	<p>The well documented study is indicating the same boiling point as the handbook data. Furthermore the following references could be found:</p> <ul style="list-style-type: none">• GDL Database: :

	<p>Value = 97.4 deg C, 101.3 kPa</p> <p>Source: D'Ans-Lax; 4. Auflage (1983)</p> <ul style="list-style-type: none"> • HSDB Database <p>Value: 97.2 deg C</p> <p>Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1348]</p> <p>In this case the given values are all about the value of 97.2 °C.</p> <p>Additional in the study the ebulliometer method was used which is one of the indicated methods in EU A.2. Due to the fact that the study is older the result is confirmed with the further references we found.</p> <p>Therefore we decided that the given data for the boiling point are acceptable.</p> <p>The correct quotation for the following field entries of the Boiling points are:</p> <p><u>Boiling Point 1:</u></p> <p>Method: In accordance with 92/69/EEC A.2, Ebbuliometer Purity: 99.94 %; No specification data Remarks/Justification: This is an accepted Handbook data without information about the specification. GLP: No</p> <p><u>Boiling Point 2:</u></p> <p>Purity: 99.9 %; No specification data Remarks/Justification: This is an accepted Handbook data without information about the method and the specification. GLP: No The field entry of Method should be deleted.</p> <p><u>Boiling Point 3 and 4:</u></p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No The field entries of Method and Purity/Specification should be deleted.</p>
Conclusion	
Reliability	2
Acceptability	acceptable
Remarks	-
Date	2016/05/31
3.1.3 Bulk density/ relative density	For the relative density several handbook data which are indicating a value of 0.80 are stated.
Rel. density 1	Other values in/ or further references could not be found. The checked databases are all citing the already given values.
Rel. density 2	
Rel. density 3	Additionally the given specific values of the density are in the range than the relative density values.
Rel. density 4	
Rel. density 5	Thus we conclude that the given data are acceptable.
Conclusion	<p>The Annotations are related to the Rel. densities 1-5 data.</p> <p>The correct quotation for the following field entries are:</p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p>

Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2016/05/31
3.2 Vapour pressure (IIA3.2)	Two references are submitted by the applicant who are handbook data and are referenced to secondary literature. So in the first step it was checked if main information (e.g. substance, purity and method) is stated in the reference. In a second step we have done a weight of evidence assessment. During the assessment we have compared the values of several literature sources.
Vapour pressure 1	
Vapour pressure 2	Unfortunately no further values could be found. As the two handbook values are confirmed with two references which calculate the vapour pressure. We decide that the values are acceptable.
Conclusion	The Annotations are related to the vapour pressure data 1 and 2. The correct quotation for the following field entries are: Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No The calculations of the vapour pressure 3 and 4 are seen as confirming information, because a test is requested for the determination of the vapour pressure and no calculation.
Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2008/09/17
3.2.1 Henry's Law Constant (Pt. I-A3.2)	The correct quotation for the following field entries are: Remarks: The field entry should be deleted.
Henry's Law Constant 1	GLP: No
Henry's Law Constant 2	
Henry's Law Constant 3	
Conclusion	The Henry's Law Constant 3 is assumed in DocII, because the given data of the Henry's Law Constant 1 and 2 are not in the study summaries. Only dimensionless Henry's Law Constant have been measured in the given references.
Reliability	2
Acceptability	acceptable
Remarks	Based on a comment we were asked for clarification regarding the two different values of the Henry's Law constant. As mentioned above the values 1 and 2 were not considered relevant as the stated values could not be found in the reference and no information about the calculation was submitted. The applicant stated this issue in his answer and submitted a further reference which supports the value of 0,75 of Sander et al and the episuite calculation.
Date	2008/05/21
3.3.1 Physical state	The correct quotation for the following field entries are: Purity: n-propanol pure Result: liquid GLP: No

Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The field entry of method should be deleted because the data of a new source are amended.
Date	2008/05/21
3.3.2 Colour	The correct quotation for the following field entries are: Purity: n-propanol pure Result: colourless GLP: No Reference: SDS BASF 2006
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The field entry of method should be deleted because the data of a new source are amended.
Date	2008/05/21
3.3.3 Odour	The correct quotation for the following field entries are: Purity: n-propanol pure Result: mild, alcohol - like GLP: No Reference: SDS BASF 2006
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The field entry of method should be deleted because the data of a new source are amended.

Date	2008/09/17
3.4 Absorption spectra (IIA3.4) UV/VIS	<p>The following Annotations related to the data of Lysoform: The correct quotation for the following field entries are: Method: Spectroscopic method Purity/Specification: 99,83%, Batch: 07-00810-0-RDAM Remarks: the field entry should be deleted</p> <p>The following Annotations related to the data of BASF: The correct quotation for the following field entries are: Method: Spectroscopic method Purity/Specification: 99,93%; Batch – Nr.: Tank 288 Remarks: the field entry should be deleted</p>
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The entry for the CRC Handbook spectrum should be deleted. Spectra of the own active substance are submitted, so this spectrum is out of interest.
Date	2008/09/17
3.4 Absorption spectra (IIA3.4) IR	<p>The following Annotations related to the data of Sasol: The correct quotation for the following field entries are: Method: NaCl Purity/Specification: 99,83%, Batch: 07-00810-0-RDAM Results: 3500 cm⁻¹ (OH-vibrations) 3000 cm⁻¹ (CH-valence) Remarks: the field entry should be deleted</p> <p>The following Annotations related to the data of BASF: The correct quotation for the following field entries are: Method: KBr Purity/Specification: 99,93%; Batch – Nr.: Tank 288 Results: 3335, 2963, 2937, 2878, 1458, 1383, 1235, 1099, 1069, 1056, 1017, 969, 887, 858, 754, 661, 465 cm⁻¹ Remarks: the field entry should be deleted</p>
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The entry for the SDBS Handbook spectrum should be deleted. Spectra of the own active substance are submitted, so this spectrum is out of interest.
Date	2008/09/17
3.4 Absorption spectra (IIA3.4) NMR	<p>The following Annotations related to the data of Lysoform: The correct quotation for the following field entries are: Method: 1H – NMR, 400 MHz, DMSO Purity/Specification: 99,83%; Batch: 07-00810-0-RDAM Remarks: the field entry should be deleted</p> <p>The following Annotations related to the data of BASF: The correct quotation for the following field entries are: Method: 1H – NMR, 400 MHz, CDCl₃ Purity/Specification: 99,93%; Batch – Nr. Tank 288 Results: The proton NMR spectrum consists of the following chemical shifts, δ ppm: CH3: 0.94 (t) CH2: 1.57 (s); 3.582 (t) OH: 1.94 (s) Remarks: the field entry should be deleted</p>

Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	<p>The entry for the SDBS Handbook spectrum should be deleted. Spectra of the own active substance are submitted, so this spectrum is out of interest.</p> <p>In Doc II A "The NMR spectra confirms to the molecular structure of Propan-1-ol" will be confirm for the Sasol NMR spectra.</p>
Date	2008/09/17
3.4 Absorption spectra (IIA3.4) MS	<p>The following Annotations related to the data of Lysoform: The correct quotation for the following field entries are: Method: EI-Mode, 70 e.V, 1,35kV Purity/Specification: > 99,8% Batch: 07-00810-0-RDAM Results: M⁺ at m/z 31 CH₂OH]⁺, m/z 29 CH₃CH₂]⁺, m/z 27 CH₂CH]⁺, m/z 42 CH₃CH₂CH]⁺, m/z 60 M⁺, Remarks: the field entry should be deleted</p> <p>The following Annotations related to the data of BASF: The correct quotation for the following field entries are: Method: EI-Mode, 70 e.V Purity/Specification: 99,93%; Batch – Nr. Tank 288 Results: M⁺ at m/z 31 CH₂OH]⁺, m/z 29 CH₃CH₂]⁺, m/z 27 CH₂CH]⁺, m/z 42 CH₃CH₂CH]⁺, m/z 60 M⁺, Remarks: the field entry should be deleted</p>
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The entry for the CRC Handbook spectrum should be deleted. Spectra of the own active substance are submitted, so this spectrum is out of interest.
Date	2016/05/31
3.5 Solubility in water (IIA3.5)	Two handbook data which indicate that propan-1-ol is indefinitely soluble in water are submitted. Additional to these the following references could be found:
Water solubility 1	
Water solubility 2	<ul style="list-style-type: none">• EU RAR: : Value = completely soluble Source: Yaws et al. (1990)• HSDB Database Value: 1.00X10+6 @ 25 deg C Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 194• GDL Database: : Value = completely soluble Source: D'Ans-Lax; 4. Auflage (1983) <p>Based on the same value stated in several literature data we accepted this data and required no further information or a test.</p>
Conclusion	<p>The Annotations are related to the water solubility data 1 und 2. The correct quotation for the following field entries are: Remarks/Justification: This is an accepted Handbook data without information</p>

Reliability	about the method, the purity and the specification. GLP: No 2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2008/07/04
3.6 Dissociation constant (-)	The correct quotation for the following field entries is: Remarks: Please refer to the additional justification. The field entries of Results, GLP and Reliability should be deleted
Conclusion	-
Reliability	-
Acceptability	acceptable
Remarks	-
Date	2008/03/17
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	The correct quotation for the following field entries are: Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2008/07/04
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)	The correct quotation for the following field entries is: Remarks: Please refer to the additional justification. The field entries of Results, GLP and Reliability should be deleted
Conclusion	-
Reliability	-
Acceptability	acceptable
Remarks	-
Date	2016/05/31
3.9 Partition coefficient n-octanol/water (IIA3.6) log P _{OW} 1	Three literature references are submitted for the Log Pow. Additional to these references in the EU RAR several values between 0.25 and 0.38 are stated. These values of safety data sheets without further information and calculated values like 0.271 (according to Rekker with program PRO-LOGP, ver.2 from CompuDrug Ltd.). Additional the following databases are stating: <ul style="list-style-type: none">• HSDB Database Value: 0.25 Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American

	<p>Chemical Society., 1995., p. 7</p> <ul style="list-style-type: none"> Ineris: Value = 0.34 Source: ECB; EU RAR Value = 0.25 Source: US EPA (2011); EPI suite tool 4.0 <p>The given method for log Pow could not be verified.</p> <p>Additional in the EU-Method A.8 calculation is recommended if the experimental methods are not available.</p> <p>Hence the calculated and the experimental methods results in the same values (range 0.25 – 0.34) the submitted literature data is acceptable.</p>
Conclusion	<p>The correct quotation for the following field entries are:</p> <p><u>log P_{ow} 1:</u> Method: in accordance with 92/69/EEC A.8 (shaking flask method) Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No The field entry of Purity/Specification should be deleted.</p> <p><u>log P_{ow} 2:</u> Results: result: 0.25 temperature: - pH: - (measured) Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No The field entries of Method and Purity/Specification should be deleted. The pH-value was not given in the literature, so it was deleted.</p> <p><u>log P_{ow} 3:</u> Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No The shake flask method could not be identified in the given literature.</p>
Reliability	2
Acceptability	acceptable
Remarks	The field entry of Purity/Specification should be deleted.
Date	2008/03/17
3.9 Partition coefficient n-octanol/water (IIA3.6)	<p>The correct quotation for the following field entries are:</p> <p>Results: result: 0.25 temperature: - pH: - (measured)</p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p>
Conclusion	-

Reliability	2
Acceptability	acceptable
Remarks	-
Date	2017/03/17
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	Handbook data for the auto-ignition temperature (liquids and gases) were provided. Justifications for non-submission of data are missing for following hazard classes: <ul style="list-style-type: none">- Flammability in contact with water- Pyrophoric properties
Conclusion	Recommended Auto-ignition temperatures (liquids and gases): 385 °C (pure), method: EU method A.15 (DIN 51794) ¹⁾ From the structural formula and composition of the substance it can be concluded that the substance does not evolve any flammable gases in contact with water or humid air and that the substance is stable at room temperature air and is not pyrophoric.
Reliability	2
Acceptability	Acceptable
Remarks	1) CHEMSAFE reference: Database that contains safety characteristic data for fire and explosion prevention, evaluated and recommended by experts at BAM and PTB. CHEMSAFE is a joint project between BAM (Berlin), PTB (Braunschweig) and DECHEMA (Frankfurt am Main), 2016
Date	2017/03/17
3.12 Flash-point (IIA3.9)	Handbook data for the flash-point were provided. Valid data for the flash-point are necessary for the classification according to Regulation (EC) No 1272/2008.
Conclusion	We recommended following flash-points: 22 °C (Impurity: iso-propanol, commercial n-propanol), method: closed cup 23.5 °C (Propan-1-ol: 99.9 %), closed cup method: DIN 51755, ISO 3679 corrected, recommended value ¹⁾
Reliability	2
Acceptability	Acceptable
Remarks	1) CHEMSAFE reference: Database that contains safety characteristic data for fire and explosion prevention, evaluated and recommended by experts at BAM and PTB. CHEMSAFE is a joint project between BAM (Berlin), PTB (Braunschweig) and DECHEMA (Frankfurt am Main), 2016
Date	2016/05/31
3.13 Surface tension (IIA3.10)	The applicant submitted three references for the surface tension. The first two references are stating values for pure Propan-1-ol.
Surface tension 1	The third one states a value for 0.1 % solution with is equal to 1g/L. This concentration of the test solution is in accordance with EG 440/2008 A.5 and the Guidance on the Biocidal Products Regulation. The value of 67.1 mN/m at 25 °C with c= 1g/L is also cited in the EU RAR.
	As the correct concentration of the test solution is used the information of Log Pow 3 are seen as acceptable and will be assumed in Doc II,
Conclusion	The correct quotation for the following field entries are:

	<p><u>Surface tension 1:</u></p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p> <p><u>Surface tension 2:</u></p> <p>Method: EC Directive 92/69 EEC, A.5 (Surface tension), plate method. Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p> <p><u>Surface tension 3:</u></p> <p>Result: result: 67.1 mN/m; temperature: 25 °C; concentration 1g/L Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p> <p>The field entries of Method and Purity/Specification should be deleted.</p>
Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2008/03/17
3.14 Viscosity (-)	<p>The correct quotation for the following field entries are:</p> <p>Results: result: 1.945 mPa • s temperature: 25 °C</p> <p>result: 1.107 mPa • s temperature: 50 °C</p> <p>Remarks/Justification: This is an accepted Handbook data without information about the method, the purity and the specification. GLP: No</p>
Conclusion	-
Reliability	2
Acceptability	acceptable
Remarks	The field entries of Method and Purity/Specification should be deleted.
Date	2016/05/25
3.15 Explosive properties (IIA3.11)	Justification for non-submission of data was not provided. However, the term "lower explosion limit" (LEL) refers to explosive atmosphere and is not subject to EU method A.14. The active substance has no explosive properties.
Conclusion	No explosive properties due to structural reasons.
Reliability	4
Acceptability	Acceptable
Remarks	-
	COMMENTS FROM OTHER MEMBER STATE (<i>specify</i>)
Date	<i>Give date of comments submitted</i>
Results and discussion	<i>Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion. Discuss if deviating from view of rapporteur member state</i>
Conclusion	<i>Discuss if deviating from view of rapporteur member state</i>

Reliability

Discuss if deviating from view of rapporteur member state

Acceptability

Discuss if deviating from view of rapporteur member state

Remarks


Section A3.6 Dissociation constant

Annex Point IIA3

JUSTIFICATION FOR NON-SUBMISSION OF DATA		Official use only
Other existing data []	Technically not feasible []	Scientifically unjustified [X]
Limited exposure []	Other justification [X]	
Detailed justification:	Expert judgement: <div style="background-color: black; width: 100%; height: 15px; margin-bottom: 5px;"></div> <div style="background-color: black; width: 100%; height: 15px; margin-bottom: 5px;"></div>	
References:	None	

Evaluation by Competent Authorities	
Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	2008/07/04
Evaluation of applicant's justification	Applicant's justification is adopted
Conclusion	acceptable
Remarks	-
COMMENTS FROM OTHER MEMBER STATE <i>(specify)</i>	
Date	<i>Give date of comments submitted</i>
Evaluation of applicant's justification	<i>Discuss if deviating from view of rapporteur member state</i>
Conclusion	<i>Discuss if deviating from view of rapporteur member state</i>
Remarks	
Reliability	<i>Discuss if deviating from view of rapporteur member state</i>
Acceptability	<i>Discuss if deviating from view of rapporteur member state</i>
Remarks	

Section A3.8
Annex Point IIA3.2Stability in organic solvents used in b.p. and identity of
relevant breakdown products

JUSTIFICATION FOR NON-SUBMISSION OF DATA		Official use only
Other existing data []	Technically not feasible []	Scientifically unjustified [X]
Limited exposure []	Other justification [X]	
Detailed justification:	Expert judgement: 	
References:	None	

Evaluation by Competent Authorities	
Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	2008/07/04
Evaluation of applicant's justification	applicant's justification is adopted
Conclusion	acceptable
Remarks	-
COMMENTS FROM OTHER MEMBER STATE (specify)	
Date	Give date of comments submitted
Evaluation of applicant's justification	Discuss if deviating from view of rapporteur member state
Conclusion	Discuss if deviating from view of rapporteur member state
Remarks	
Reliability	Discuss if deviating from view of rapporteur member state
Acceptability	Discuss if deviating from view of rapporteur member state
Remarks	

Section A3.10 Thermal stability, identity of relevant breakdown products
Annex Point IIA3.7

JUSTIFICATION FOR NON-SUBMISSION OF DATA

Official use only

Other existing data [] Technically not feasible [] Scientifically unjustified [X]
Limited exposure [] Other justification [X]

Detailed justification:

Expert judgement:

[REDACTED]

References:

None

Evaluation by Competent Authorities

Use separate "evaluation boxes" to provide transparency as to the comments and views submitted

EVALUATION BY RAPPORTEUR MEMBER STATE

Date 2010/02/03
Evaluation of applicant's justification Applicant's justification is adopted
Conclusion acceptable
Remarks -

COMMENTS FROM OTHER MEMBER STATE (specify)

Date Give date of comments submitted
Evaluation of applicant's justification Discuss if deviating from view of rapporteur member state
Conclusion Discuss if deviating from view of rapporteur member state
Remarks

Reliability Discuss if deviating from view of rapporteur member state
Acceptability Discuss if deviating from view of rapporteur member state
Remarks

Section A3.16 Oxidizing properties


Annex Point IIA3.12

JUSTIFICATION FOR NON-SUBMISSION OF DATA		Official use only
Other existing data []	Technically not feasible []	Scientifically unjustified [X]
Limited exposure []	Other justification [X]	
Detailed justification:	Expert judgement: <div style="background-color: black; width: 100%; height: 15px; margin-bottom: 5px;"></div> <div style="background-color: black; width: 100%; height: 15px; margin-bottom: 5px;"></div>	
References:	None	

Evaluation by Competent Authorities	
Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	2008/07/04
Evaluation of applicant's justification	Applicant's justification is adopted
Conclusion	acceptable
Remarks	-
COMMENTS FROM OTHER MEMBER STATE (specify)	
Date	<i>Give date of comments submitted</i>
Evaluation of applicant's justification	<i>Discuss if deviating from view of rapporteur member state</i>
Conclusion	<i>Discuss if deviating from view of rapporteur member state</i>
Remarks	
Reliability	<i>Discuss if deviating from view of rapporteur member state</i>
Acceptability	<i>Discuss if deviating from view of rapporteur member state</i>
Remarks	

Section A3.17 Reactivity towards container material

Annex Point IIA3.13

JUSTIFICATION FOR NON-SUBMISSION OF DATA		Official use only
Other existing data []	Technically not feasible []	Scientifically unjustified [X]
Limited exposure []	Other justification [X]	
Detailed justification:	Expert judgement:	X
		
References:	None	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	2010/02/03
Evaluation of applicant's justification	Applicant's justification is adopted
Conclusion	acceptable
Remarks	Suitable container materials are e. g. PE-HD and austenitic steels (products have to be free from chlorides and bromides). (PVC e. g. is not compatible with propanol)
COMMENTS FROM OTHER MEMBER STATE (specify)	
Date	Give date of comments submitted
Evaluation of applicant's justification	Discuss if deviating from view of rapporteur member state
Conclusion	Discuss if deviating from view of rapporteur member state
Remarks	
Reliability	Discuss if deviating from view of rapporteur member state
Acceptability	Discuss if deviating from view of rapporteur member state
Remarks	