Ethylene Oxide

For use as a gaseous sterilant (PT2)

Document IIIA

Section 3

Physical and chemical properties

March 2020

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Please refer to "Technical Notes for Guidance on Dossier Preparation including preparation and evaluation of study summaries under Directive 98/8 EC Concerning the Placing of Biocidal Products on the Market (Appendix 7.1 and 7.2)" for a list of the Standard Terms and Abbreviations used in this document.

Section A3	**3. 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 (IIA 3.1)								
3.1.1 Melting point	Not documented	Pure, assumed >99%	-112.5ºC		N	0	Lide, 2005, CRC handbook	
3.1.2 Boiling point	Not documented	Pure, assumed >99%	11ºC		N	0	Verschueren 1983	
3.1.3 Bulk density/ relative density								
	Not documented	Pure, assumed >99%	Density 0.8821[10] g/cm^3		N	0	Lide, 2005, CRC handbook (pg. 568)	x
3.2 Vapour pressure (IIA 3.2)	Not documented	Pure, assumed >99%	146 kPa at 20°C		N	0	Verschueren 1983	
3.2.1 Henry's Law Constant (Pt. I-A3.2)	Calculation	-	14 Pa m^3 mol^{-1}	Calculated from activity coefficient and vapor pressure presented Conway et al., 1983	N	3	BUA 1995; Conway et al., 1983	
3.3 Appearance (IIA 3.3)								

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3.3.1 Physical state	Not documented	Pure, assumed >99%	Gas (at 25°C and normal atmospheric pressure).		N	0	Merck 2001	
3.3.2 Colour	Visual assessment	Pure, assumed >99%	Colourless		N	0	Verschueren 1983	
3.3.3 Odour	Not documented	Pure, assumed >99%	Sweet, olefinic		N	0	Verschueren 1983	
3.4 Absorption spectra (UV/VIS, IR, NMR) and a mass spectrum, molar extinction at relevant wavelengths, where relevant (IIA 3.4)								
3.4.1 UV/VIS	Not documented	Pure, assumed >99%	Absorbance maxima at159 nm, 171 nm and 174 nm.		N	0	NIST (2009a)	
3.4.2 IR	Not documented	Pure, assumed >99%	Maxima at 850 microns, 1275 microns and 3025 microns		N	0	NIST (2009b) [Data from Coblentz Society 1973]	
3.4.3 NMR	Not documented	Pure, assumed >99%	Spectra was recorded at 10 mole % concentration. Three		N	3	Gazzard, I.J. (1971)	

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			groups of maxima peaks were obtained with an observed symmetry that confirmed the molecular geometry.					
3.4.4 MS	Not documented	Pure, assumed >99%	Major MS fragment m/z 29 (base peak= 1.0), 44 (0.66) , 42 (0.11), 15 (0.66) (NIST, 1998)		N	0	NIST/EPA/NIH (2009c)	
3.5 Solubility in water (IIA 3.5)	Not documented	Pure, assumed >99%	1000 g/L at 25ºC		N	0	Merck 2001	
3.6 Dissociation constant (-)	-	-	-	Ethylene oxide does not contain any dissociation groups	-	-	-	
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA 3.1)	Not documented	Pure, assumed >99%	Soluble in alcohol and ether		N	0	Merck 2001	
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA 3.2)	-	-	-	Ethylene oxide is not used in organic solvents	-	-	-	

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3.9 Partition coefficient n-octanol/water including effect of pH (5 to 9) and temperature (IIA 3.6)	Not documented	Pure, assumed >99%	Log P_{OW} = -0.3		N	3	Hansch and Leo, 1979	
3.10 Thermal stability, identity of relevant breakdown products (IIA 3.7)	-	-	Ethylene oxide is not an endothermic molecule and cannot decompose exothermically into its elements. However it can decompose or polymerise exothermically into various distributions of more stable products.		N	3	Britton, LG (1990)	
3.11 Flammability, including auto-flammability and identity of combustion products (IIA 3.8)	Not documented	Pure, assumed >99%	Flammable limits of 3 to 100% in ambient air		N	3	Britton, LG (1990)	
	Not documented	Pure, assumed >99%	Auto ignition temperature 457ºC		N	3	Britton, LG (1990)	
3.12 Flash-point (IIA 3.9)	-	-	-	EtO is a gas at room temperature, and therefore the flash point consequently has no relevance under BPR, however flash points of -29 °C are reported in	-	-	-	

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				the technical literature. In any case, testing is not technically possible for Ethylene oxide as it is explosive under certain conditions and pyrophoric. (See Appendix II)				
3.13 Surface tension (IIA 3.10)	-	-	-	Ethylene oxide is too hazardous to be experimentally determined for surface tension. Based on chemical structure, no surface activity is predicted. (see Appendix II)	-	-	-	
3.14 Viscosity (-)	-	-	-	Viscosity is required for liquid substances determined at 20 and 40 °C. Ethylene oxide is a gas at 20 and 40 °C, therefore determination of viscosity by test	-	-	-	

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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**
				method OECD 114 is not possible. (See Appendix II)				
3.15 Explosive properties (IIA 3.11)	Not documented	Pure, assumed >99%	Ethylene oxide is classed as explosive		N	0	Merck 2001	
3.16 Oxidizing properties (IIA 3.12)	-	-	-	Based on handling experience and historical use, ethylene oxide is not oxidising. (See Appendix II)	-	-	-	
3.17 Reactivity towards container material (IIA 3.13)	Not documented	Pure, assumed >99%	Ethylene oxide reacts with water, strong acids, alkalis, and oxidizers; chlorides of iron, tin, and aluminium; and oxides of iron and aluminium. Based on experience, suitable materials for ethylene oxide are: Normalised steel and carbon steel, tempered steel, aluminium alloys, stainless steel.		N	0	Supporting information: ATSDR MMG 2007a; IPCS EHC 55	

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Summary and Conclusions

The physical and chemical properties of ethylene oxide are well documented in public domain literature and some reputable sources together with existing data reviews have been used to summarise the annex points presented above.

Ethylene oxide is a colourless gas at standard room temperature and pressure. It is a colourless liquid under 10.7°C or when stored under pressure. It has a high vapour pressure and is fully miscible in water, therefore having a very high water solubility. It is an extremely flammable gas at concentrations between 3 and 100% in air. It is explosive in air concentrations of greater than 3%. It is very reactive in both the liquid and vapour phases.

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	Evaluation by Rapporteur Member State
Date	March 2020
Materials and methods	Not relevant
Conclusion	Taking the remarks below into consideration, the physico-chemical data for ethylene oxide is deemed to be acceptable.
Reliability	Not applicable
Acceptability	Acceptable
Remarks	*Comment to the use of reliability index: As almost all physico-chemical data for ethylene oxide is taken from open literature or handbooks it seems inappropriate to assign a reliability index. These endpoints are given a reliability index of 0. Endpoints taken from literature other than handbooks, or peer reviewed publications, are given a reliability of 3. Specific remarks: 3.1.3 – The correct density is 0.8821 g/cm^3 at 10 ^{o}C. A general remark to all endpoints: Ethylene oxide is generated from very pure starting materials in a relatively simple catalytic and solvent free process. The process involves only the two reactants (gases) and a solid phase catalyst. Furthermore, ethylene oxide is a gas at room temperature, but condenses at approximately 10 degrees Celsius, which makes for simple and effective clean up by distillation/condensation. None of the foreseen impurities, nor any of the starting materials, are likely to have a boiling point close to the boiling point of ethylene oxide. It is therefore expected that the ethylene oxide used for the physico-chemical testing is of high purity. Furthermore, ethylene oxide is a well-known and well documented substance. It is included in both the CRC handbook of physics and chemistry and The Merck Index. The eCA therefore, finds no reason to doubt the data submitted. All studies submitted for the physico-chemical properties of ethylene oxide are from open domain literature. Most of which are handbooks, not stating the purity of substance tested, or the method used for testing. Some sources other than handbooks have been accepted. However, some of them are given a reliability score of 3 and are only used as supplementary data. The data needed for assessment of (eco)toxicological properties has been deemed acceptable by the (eco)toxicological experts, and no further data will be requested by the eCA. Some hazard classes are not applicable to gases. Please see the CAR for the correct physical hazard classification of ethylene oxide.

Appendix I

Data waiver forms.

Section 3 **Annex IIA Point 3.9**	**3.12 Flash point**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA *As outlined in the TNsG on data requirements, the applicant must always be able to justify the suggested exemptions from the data requirements. The justifications are to be included in the respective location (section) of the dossier.* *If one of the following reasons is marked, detailed justification has to be given below. General arguments are not acceptable*	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [x]** **Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	EtO is a gas at room temperature, and therefore the flash point consequently has no relevance under BPR, however flash points of -29 °C are reported in the technical literature. In any case, testing is not technically possible for Ethylene oxide as it is explosive under certain conditions and pyrophoric.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	March 2020	
Evaluation of applicant's justification	-	
Conclusion	Acceptable	
Remarks		

Section 3 **Annex IIA Point 3.10**	**3.13 Surface Tension**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA *As outlined in the TNsG on data requirements, the applicant must always be able to justify the suggested exemptions from the data requirements. The justifications are to be included in the respective location (section)*	Official use only

Section 3 **Annex IIA Point 3.10**	**3.13 Surface Tension**	
	of the dossier. *If one of the following reasons is marked, detailed justification has to be given below. General arguments are not acceptable*	
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [x]** **Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Ethylene oxide is too hazardous to be experimentally determined for surface tension. Based on chemical structure, no surface activity is predicted. This was concluded in the REACH dossier for ethylene oxide https://echa.europa.eu/registration-dossier/-/registered-dossier/15813/4/11	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	March 2020	
Evaluation of applicant's justification		
Conclusion	Acceptable, with remark	
Remarks	Surface tension is not required for the ecotoxicological assessment of ethylene oxide.	

Section 3 **Annex IIIA Point 3.14**	**3.14 Viscosity**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA *As outlined in the TNsG on data requirements, the applicant must always be able to justify the suggested exemptions from the data requirements. The justifications are to be included in the respective location (section) of the dossier.* *If one of the following reasons is marked, detailed justification has to be given below. General arguments are not acceptable*	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Viscosity is required for liquid substances determined at 20 and 40 °C. Ethylene oxide is a gas at 20 and 40 °C, therefore	

Section 3 **Annex IIIA Point 3.14**	**3.14 Viscosity**	
	determination of viscosity by test method OECD 114 is not possible.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	March 2020	
Evaluation of applicant's justification	-	
Conclusion	Acceptable	
Remarks		

Section 3 **Annex IIIA Point 3.16** **(Annex IIA 3.12)**	**3.16 Oxidising**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA *As outlined in the TNsG on data requirements, the applicant must always be able to justify the suggested exemptions from the data requirements. The justifications are to be included in the respective location (section) of the dossier.* *If one of the following reasons is marked, detailed justification has to be given below. General arguments are not acceptable*	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [ ]** **Other justification [x]**	
Detailed justification:	Ethylene oxide was considered for classification as an oxidising gas with respect to the CLP guidance and ISO 10156:2017. It is noted in the CLP guidance (Guidance on the Application of the CLP Criteria Version 5.0 – July 2017): "There are not many pure gases that are oxidising. Most oxidising gases are identified as such in the UN RTDG Model Regulations and in ISO 10156 Gases and gas mixtures: Determination of fire potential and oxidizing ability for the selection of cylinder valve outlets as amended." Ethylene oxide is considered to be a pure gas as purity as manufactured is >99%. Furthermore, ethylene oxide is not noted to be a known oxidising gas in ISO 10156:2017, hence coefficient of oxygen equivalency data is not available for the calculation method. Therefore, based on ISO 10156:2017, handling experience and historical use, ethylene oxide is not oxidising.	

Section 3 **Annex IIIA Point 3.16** **(Annex IIA 3.12)**	**3.16 Oxidising**
Undertaking of intended data submission [ ]	
	Evaluation by Competent Authorities
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	March 2020
Evaluation of applicant's justification	-
Conclusion	Acceptable.
Remarks	Ethylene oxide has a harmonised classification. According to the harmonised classification, ethylene oxide is not an oxidising gas.