

# ***European Commission***



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

## **Mecoprop-P** **Volume 3 – B.2 (AS)**

**Rapporteur Member State : United Kingdom**  
**Co-Rapporteur Member State : Ireland**

## **Version History**

<b>When</b>	<b>What</b>
31/03/2016	Initial Renewal Assessment Report (RAR)

## Table of contents

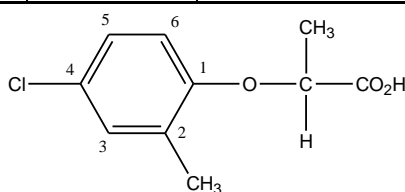
<b><u>B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE</u></b> .....	4
<b><u>B.2.1. MELTING POINT AND BOILING POINT</u></b> .....	4
<b><u>B.2.2. VAPOUR PRESSURE, VOLATILITY</u></b> .....	4
<b><u>B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)</u></b> .....	5
<b><u>B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY</u></b> .....	5
<b><u>B.2.5. SOLUBILITY IN WATER</u></b> .....	8
<b><u>B.2.6. SOLUBILITY IN ORGANIC SOLVENTS</u></b> .....	8
<b><u>B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER</u></b> .....	9
<b><u>B.2.8. DISSOCIATION IN WATER</u></b> .....	9
<b><u>B.2.9. FLAMABILITY AND SHELF-HEATING</u></b> .....	9
<b><u>B.2.10. FLASH POINT</u></b> .....	10
<b><u>B.2.11. EXPLOSIVE PROPERTIES</u></b> .....	10
<b><u>B.2.12. SURFACE TENSION</u></b> .....	10
<b><u>B.2.13. OXIDISING PROPERTIES</u></b> .....	10
<b><u>B.2.14. OTHER STUDIES</u></b> .....	10
<b><u>B.2.15. SUMMARY OF PHYSICAL AND CHEMICAL PROPERTIES OF ACTIVE SUBSTANCE</u></b> .....	11
<b><u>B.2.16. REFERENCES RELIED ON</u></b> .....	12

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

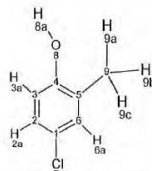
<b>Previous evaluation:</b>	None; All of the data studies referenced in the following table were submitted for the purpose of renewal under Regulation 844/2012. These replace the original annex I data that were owned by BASF (no longer supporting mecoprop-P).
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Test 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>						
Melting, freezing or solidification point B.2.1/01	EEC A1 OPPTS 830.7200	Mecoprop-P pure 99.8 % w/w	Melting point 93.5 - 97.5°C	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
Boiling point B.2.1/02	EEC A2 OPPTS 830.7220	Mecoprop-P pure 99.8 % w/w	Boiling point could not be determined. Decomposes above 240°C without boiling	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
Decomposition Sublimation temperature B.2.1/03	EEC A2 OPPTS 830.7220	Mecoprop-P pure 99.8 % w/w	Decomposes above 240°C without boiling	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
<b>B.2.2. VAPOUR PRESSURE, VOLATILITY</b>						
Vapour pressure B.2.2/01	EEC A4 OPPTS 830.7950	Mecoprop-P pure 99.8 % w/w	$1.4 \times 10^{-3}$ Pa at 25°C	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
Volatility (Henry's Law constant) B.2.2/02	Estimated from vapour pressure and water solubility (20°C)	Mecoprop-P pure 99.8 % w/w	Henry's Law Constant = $1.7 \times 10^{-4}$ Pa.m <sup>3</sup> mol <sup>-1</sup>	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)

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	OPPTS 830.6302	Mecoprop-P pure 99.8 % w/w	White solid at 20°C N 9.25/84.2% R on Munsell Colour system	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)																																						
	OPPTS 830.6303	Mecoprop-P TGAI	Dark cream solid at 20°C 2.5Y 9/2 on Munsell Colour system			Comb, A.L. NUF002/993274 (2000b)																																						
B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY																																												
Ultraviolet/visible (UV/VIS) B.2.4/01		Mecoprop-P pure 99.8 % w/w	UV (distilled water, 0.1M HCL and 0.1 M NaOH) of 29.3 mg/L and 147 mg/L solutions from 220 – 800 nm: No maxima > 400 nm. Absorptions over 220 – 400 nm reported below:	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)																																						
			<table><tr><th>Solvent</th><th>Conc. (mg/L)</th><th>λmax (nm)</th><th>Absorbance</th><th>ε (dm³/mol/cm)</th></tr><tr><td rowspan="3">Distilled water</td><td rowspan="3">29.3 147</td><td>229</td><td>1.302</td><td>9530</td></tr><tr><td>280</td><td>1.005</td><td>1470</td></tr><tr><td>285 (sh)</td><td>0.879</td><td>1290</td></tr><tr><td rowspan="3">0.1M HCL</td><td rowspan="3">29.3 147</td><td>227</td><td>1.210</td><td>8860</td></tr><tr><td>279</td><td>0.916</td><td>1340</td></tr><tr><td>284 (sh)</td><td>0.797</td><td>1770</td></tr><tr><td rowspan="3">0.1M NaOH</td><td rowspan="3">29.3 147</td><td>229</td><td>1.300</td><td>9520</td></tr><tr><td>280</td><td>1.065</td><td>1560</td></tr><tr><td>286 (sh)</td><td>0.930</td><td>1360</td></tr></table>				Solvent	Conc. (mg/L)	λmax (nm)	Absorbance	ε (dm³/mol/cm)	Distilled water	29.3 147	229	1.302	9530	280	1.005	1470	285 (sh)	0.879	1290	0.1M HCL	29.3 147	227	1.210	8860	279	0.916	1340	284 (sh)	0.797	1770	0.1M NaOH	29.3 147	229	1.300	9520	280	1.065	1560	286 (sh)	0.930	1360
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Infrared (IR) B.2.4/02		Mecoprop-P pure 99.8 % w/w	IR (KBr disc) 4000 – 500 cm <sup>-1</sup>	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)																																						

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results			Comments (Acceptable / Non acceptable)	GLP	Reference						
			Frequency (cm <sup>-1</sup> )	Observation	Assignment									
			2500 - 3500	Broad, medium band	O-H stretch (H-bonded)									
			3037	Weak, sharp band	C-H (aromatic) stretch									
			2840 – 3000	Weak, sharp bands	C-H (alkyl) stretches									
			1710	Strong, sharp band	C=O stretch (H-bonded)									
			1200 – 1600	Strong, sharp bands	Region includes: C-C (aromatic) stretch CH <sub>3</sub> deformations C-OH in plane deformation									
			1000 – 1200	Medium, sharp bands	Region includes: C-H (aromatic) in plane deformation C-O-C stretch									
			<1000	Weak, sharp bands	Region includes: C-H (aromatic) out of plane deformation C-OH out of plane deformation Skeletal vibrations									
Nuclear magnetic resonance (NMR) B.2.4/03		Mecoprop-P pure 99.8 % w/w	<div></div> <p><sup>1</sup>H-NMR (250 MHz, CDCl<sub>3</sub>)</p> <table><tr><th>δ (ppm) relative to TMS</th><th>Assignment</th></tr><tr><td>8.1</td><td>CO<sub>2</sub><u>H</u></td></tr><tr><td>7.26</td><td>Solvent</td></tr></table>			δ (ppm) relative to TMS	Assignment	8.1	CO <sub>2</sub> <u>H</u>	7.26	Solvent	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
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8.1	CO <sub>2</sub> <u>H</u>													
7.26	Solvent													

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results			Comments (Acceptable / Non acceptable)	GLP	Reference	
			7.14	<u>H</u> -C <sup>3</sup>					
			7.07	<u>H</u> -C <sup>5</sup>					
			6.63	<u>H</u> -C <sup>6</sup>					
			4.75	CH <sub>3</sub> <u>C</u> H					
			2.24	C <u>H</u> <sub>3</sub> -C <sup>2</sup>					
			1.67	C <u>H</u> <sub>3</sub> CH					
Mass spectra (MS) B.2.4/04		Mecoprop-P pure 99.8 % w/w	MS (EI)			Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)	
			Peak - m/z	Assignment					
			214	molecular ion					
			169	loss of COOH from molecular ion					
			142	loss of CHCH <sub>3</sub> from m/z = 169 fragment					
Spectra for impurities B.2.4/05		4-chloro-2-methylphenol (IMP-5, PCOC) 96.61 % w/w	UV (water, 200 – 800 nm)				Acceptable.	N	Calvert, A. AC529/45 (2010) and Calvert, A. 2015c
			Solvent (pH)	Conc. (mg/L)	λmax (nm)	Absorbance			
			Dilute HCl (4.06)	57.2	226.2 280.0	3.000 0.682			
			Water (7.02)	57.2	228.8 279.0	2.617 0.683			
			Dilute NaOH (8.92)	57.2	229.0 280.6	2.476 0.661			
			IR (KBr disc) 4000 – 600 cm <sup>-1</sup> : 3247.2 (OH stretch); 1498.7, 1451.4 and 1405.9 (sp <sup>2</sup> aryl CC str); 1241.9, 1175.9, 1119.3 (sp <sup>2</sup>						

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference																														
			<p>aryl-H in plane bend); 815.4, 805.6 (aryl C-H bend); 653.5 (C-Cl stretch).</p> <p>GC-MS, m/z = 142 [M+], 107 [C<sub>7</sub>H<sub>7</sub>O+], 77 [C<sub>6</sub>+], 51.</p> <p>NMR (<sup>1</sup>H, CDCl<sub>3</sub>):</p> <div></div> <table><thead><tr><th>Chemical Shift (PPM)</th><th>Number of Protons</th><th>Splitting</th><th>Proton Type</th><th>Assignment</th></tr></thead><tbody><tr><td>7.07</td><td>1</td><td>multiplet</td><td>Aryl H</td><td>3a</td></tr><tr><td>7.04</td><td>1</td><td>multiplet</td><td>Aryl H</td><td>2a</td></tr><tr><td>6.72</td><td>1</td><td>Doublet (J 8.48)</td><td>Aryl H</td><td>6a</td></tr><tr><td>4.75</td><td>1</td><td>singlet</td><td>O-H</td><td>8a</td></tr><tr><td>2.28</td><td>3</td><td>singlet</td><td>-CH<sub>3</sub></td><td>9a,9b,9c</td></tr></tbody></table>	Chemical Shift (PPM)	Number of Protons	Splitting	Proton Type	Assignment	7.07	1	multiplet	Aryl H	3a	7.04	1	multiplet	Aryl H	2a	6.72	1	Doublet (J 8.48)	Aryl H	6a	4.75	1	singlet	O-H	8a	2.28	3	singlet	-CH <sub>3</sub>	9a,9b,9c			
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B.2.5. SOLUBILITY IN WATER																																				
Solubility in water B.2.5/01	EEC A6 OPPTS 830.7840	Mecoprop-P pure 99.8 % w/w	<p>Measured at 20°C</p> <table><tr><td>Purified water (pH 3)</td><td>880 mg/L</td></tr><tr><td>pH 4 buffer</td><td>6.65 g/L</td></tr><tr><td>pH 7 buffer</td><td>&gt; 250 g/L</td></tr><tr><td>pH 10 buffer</td><td>&gt; 250 g/L</td></tr></table>	Purified water (pH 3)	880 mg/L	pH 4 buffer	6.65 g/L	pH 7 buffer	> 250 g/L	pH 10 buffer	> 250 g/L	Acceptable. Active has a pKa within 2 – 12 therefore acidic and alkaline ranges tested.	Y	Comb, A.L. NUF004/993523 (2000a)																						
Purified water (pH 3)	880 mg/L																																			
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B.2.6. SOLUBILITY IN ORGANIC SOLVENTS																																				
Solubility in organic solvents B.2.6/01	CIPAC Method MT181 &	Mecoprop-P Technical 92.63% w/w	<p>Solvent solubility at 20± 1°C</p> <table><tr><td>Acetone</td><td>&gt;250 g/L</td></tr><tr><td>Dichloromethane</td><td>&gt;250 g/L</td></tr><tr><td>Ethyl acetate</td><td>&gt;250 g/L</td></tr></table>	Acetone	>250 g/L	Dichloromethane	>250 g/L	Ethyl acetate	>250 g/L	Acceptable. Solubility of > 250 g/L observed in all solvents apart from heptane (7.69 g/L).	Y	Wilson, I, 14/0866 (2014)  Wilson, I., 2015																								
Acetone	>250 g/L																																			
Dichloromethane	>250 g/L																																			
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Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results		Comments (Acceptable / Non acceptable)	GLP	Reference
	modified MT157 with validated method (heptane)		Methanol	>250 g/L			15/0969 (heptane result)
			Heptane	7.69 g/L			
			Toluene	>250 g/L			
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER							
Partition coefficient n-octanol/water B.2.7/01	EEC A8 OPPTS 830.7550	Mecoprop-P pure 99.8 % w/w	Measured at 20°C pH 4 buffer log <sub>10</sub> Pow = 2.19, Pow = 156 pH 7 buffer log <sub>10</sub> Pow = -0.19, Pow = 0.64 pH 10 buffer log <sub>10</sub> Pow = -0.64, Pow = 0.23  Calculated values of log <sub>10</sub> Pow: mecoprop-P = 2.94 HMCPP = 1.47 CCPP = 1.93		Acceptable data have been provided for the active, however no test data on the plant metabolites HMCCP and CCPP have been reported in the study. Calculated values were supplied as part of a SAR analysis toxicological study (see B.2.15).	Y	Comb, A.L. NUF004/993523 (2000a)
B.2.8. DISSOCIATION IN WATER							
Dissociation constant B.2.8/01	OECD 112 OPPTS 830.7370	Mecoprop-P pure 99.8 % w/w	At 25 °C dissociation constant = 2.0 x 10 <sup>-4</sup> pKa = 3.7 (acidic)		Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
B.2.9. FLAMMABILITY AND SHELF-HEATING							
Flammability B.2.9/01	OPPTS 830.6315/ EEC A10	Mecoprop-P technical 91.5% w/w	Mecoprop-P TGAI is not flammable. At ignition, localized combustion with no spreading. Mecoprop-P charred and melted but failed to ignite.		Acceptable.	Y	Comb, A.L NUF002/993274 (2000b)
Self heating B.2.9/02	EEC 16		Mecoprop-P TGAI did not self-ignite prior to melting. No exothermic reaction of mecoprop-P technical grade below its		Acceptable.		Comb, A.L NUF002/993274

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
		Mecoprop-P technical 91.5% w	melting point at <i>ca.</i> 90 - 100°C was observed.		Y	(2000b)
<b>B.2.10. FLASH POINT</b>						
Flash point B.2.10/01	case	-	The flash point is not applicable, since Mecoprop-P is a solid.	Acceptable. Flash point not required as melting point > 40°C	-	-
<b>B.2.11. EXPLOSIVE PROPERTIES</b>						
Explosive properties B.2.11/01	EEC A14	Mecoprop-P technical 91.5% w/w	Mecoprop-P technical material is not explosive. Tests for thermal sensitivity and mechanical sensitivity (shock and friction) were negative.	Acceptable.	Y	Comb, A.L NUF002/993274 (2000b)
<b>B.2.12. SURFACE TENSION</b>						
Surface tension B.2.12/01	EEC A5	Mecoprop-P pure 99.8 % w/w	50.0 mN/m (90% saturated solution) at 20°C. As surface tension is < 60 mN/m at 20°C it is surface active.	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)
<b>B.2.13. OXIDISING PROPERTIES</b>						
Oxidizing properties B.2.13/01	EEC A17	Mecoprop-P technical 91.5% w/w	Mecoprop-P technical grade is not oxidising.	Acceptable.	Y	Comb, A.L NUF002/993274 (2000b)
<b>B.2.14. OTHER STUDIES</b>						
Relative density of purified active substance B.2.14/01	EEC A3 OPPTS 830.7300	Mecoprop-P pure 99.8 % w/w	$D_4^{22} = 1.31$	Acceptable.	Y	Comb, A.L. NUF004/993523 (2000a)

**B.2.15. SUMMARY OF PHYSICAL AND CHEMICAL PROPERTIES OF ACTIVE SUBSTANCE**

Mecoprop-P is a white solid (pure grade substance) or a dark cream solid (technical grade active substance). Mecoprop-P has a melting point of 93.5 - 97.5°C, is not flammable and has no oxidising or explosive properties. It has a relative density of 1.31 at 22°C and a vapour pressure of  $1.4 \times 10^{-3}$  Pa at 25°C. It has a solubility of > 250 g/L in water (pH 7) at 20°C and solubility of > 250 g/L in acetone, dichloromethane, ethyl acetate, methanol, toluene and 7.69 g/L in heptane at 20°C. The *n*-octanol/water partition coefficient (Log  $P_{ow}$ ) was determined to be -0.19 at pH7 and 20°C. A volatility constant (Henry's Law constant) of  $1.7 \times 10^{-4}$  Pa.m<sup>3</sup> mol<sup>-1</sup> was calculated for mecoprop-P.

The *n*-octanol/water partition coefficient is required for all components of the residue definition and therefore data on HMCPP and CCPP are necessary. The applicant submitted the following predicted values as part of a SAR analysis toxicological study to address this:

**Table A2: Toxicologically relevant physical-chemical parameters mecoprop-P and two of its metabolites (EPI Suite v4.11)**

	<b>Mecoprop-P</b>	<b>HMCPP</b>	<b>CCPP</b>
<b>SMILES</b>	<chem>CC(C(=O)=O)Oc1ccc(Cl)cc1C</chem>	<chem>CC(C(=O)=O)Oc1ccc(Cl)cc1CO</chem>	<chem>CC(C(=O)=O)Oc1ccc(Cl)cc1C(=O)=O</chem>
<b>MW</b>	214.65	230.65	244.63
<b>Vapour Pressure</b>	0.0607 Pa at 25 °C (MPBPWIN v1.43)	1.29E-05 Pa at 25 °C (MPBPWIN v1.43)	4.65E-05 Pa at 25 °C (MPBPWIN v1.43)
<b>Water Solubility</b>	282.7 mg/L at 25 °C (WSKOWWIN v1.42) 471.39 mg/L at 25 °C (WATERNT v1.01)	1.34 g/L at 25 °C (WSKOWWIN v1.42) 29.61 g/L at 25 °C (WATERNT v1.01)	1.42 g/L at 25 °C (WSKOWWIN v1.42) 5.81 g/L at 25 °C (WATERNT v1.01)
<b>Partition Coefficient</b>	log Kow 2.94 (KOWWIN v1.68)	log Kow 1.47 (KOWWIN v1.68)	log Kow 1.93 (KOWWIN v1.68)

In the absence of data these calculated parameters are considered sufficient at this stage, however test data will be required on the metabolites as confirmatory data.

**B.2.16. REFERENCES RELIED ON**

Regarding the literature search undertaken by the applicant (report dated 15/07/2015). It is considered that the search is acceptable in terms of databases searched and the search criteria applied. The search did not reveal any references of relevance to this section.

<b>Data Point</b>	<b>Author (s)</b>	<b>Year</b>	<b>Title Company 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>
CA 2.1/01 2.2/01, 2.3/01, 2.4/01, 2.5/01, 2.7/01, 2.8/01, 2.12/01 2.14/01	Comb. A.L.	2000a	Mecoprop-P (pure grade) physico-chemical properties NUF004/993523 Huntingdon Life Sciences Ltd GLP Not published	N	Y	New data submitted	Nufarm	Submitted for the purpose of renewal
CA 2.3/01, 2.9/01, 2.11/01, 2.13/01	Comb. A.L.	2000b	Mecoprop-P (technical grade) physico-chemical properties NUF002/993274 Huntingdon Life Sciences Ltd GLP Not published	N	Y	New data submitted	Nufarm	Submitted for the purpose of renewal
CA 2.4/05	Calvert , A	2015c	Identity evaluation of 4-chloro- 2-methylphenol (PCOC) produced at Nufarm UK Limited (Wyke) Updated version AC529/45 Nufarm UK Ltd Not GLP Not published	N	N	New data submitted	Nufarm	Submitted for the purpose of renewal
CA 2.6/01	Wilson. I	2014	Solubility of Mecoprop-P in Organic Solvents 14/0866 Nufarm UK Limited GLP Not published	N	Y	New data submitted	Nufarm	Submitted for the purpose of renewal
CA 2.6/02	Wilson. I	2015	Solubility of Mecoprop-P in Heptane 15/0969 Nufarm UK Limited GLP Not published	N	Y	New data submitted	Nufarm	Submitted for the purpose of renewal