Draft Assessment Report

Evaluation of Active Substances

Plant Protection Products

Prepared according to **Regulation (EC) 1107/2009**
as it applies in Great Britain (GB PPP)

Cinmethylin (BAS 684 H)

Volume 3 – B.2 (AS)
Physical &Chemical Properties

Great Britain

November 2020

Version History

When	What
November 2020)	Initial DAR

Table of contents

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

Active substance = Cinmethylin = BAS 684 H (Reg. 900202)

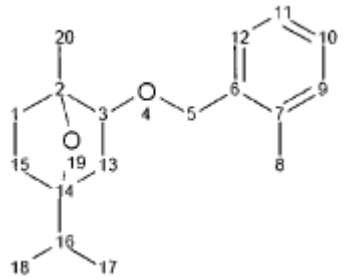
Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.1. MELTING POINT AND BOILING POINT						
Melting, freezing or solidification point **B.2.1/01**	OECD 102 (DSC)	BAS 684 H Batch No.: L2019-035 (98.6 %) COD-002494 (96.2 %)	No melting point observed. Product is liquid at room temperature. The solidification point was determined to -56 °C (pure) and -58 °C (technical material).	Acceptable. Cinmethylin is a liquid at room temperature, therefore melting point is not required.	Y	Study No.: 2019/2054650; Kroehl, T; 2019
Boiling point **B.2.1/02**	OECD 102 (DSC)	BAS 684 H Batch No.: L2019-035 (98.6 %) COD-002494 (96.2 %)	Boiling Point = 330 °C (pure) Boiling Point = 323 °C (technical material)	Acceptable	Y	Study No.: 2019/2054650; Kroehl, T; 2019
Decomposition / Sublimation temperature **B.2.1/03**	OECD 102 (DSC)	BAS 684 H Batch No.: L2019-035 (98.6 %) COD-002494 (96.2 %)	No decomposition observed up to 400 °C for either pure AS or technical material.	Acceptable	Y	Study No.: 2019/2054650; Kroehl, T; 2019
B.2.2. VAPOUR PRESSURE, VOLATILITY						
Vapour pressure **B.2.2/01**	EEC A4 OECD 104	BAS 684 H Batch No.:L87-84 (99.0 %)	Temp (°C) / Vapour Pressure (Pa) 20 / 8.1×10^{-3} 25 / 1.5×10^{-2}	Acceptable	Y	Study No.: 2015/1257674; Daum, A; 2015
Volatility (Henry's Law constant) **B.2.2/02**	Calculation	BAS 684 H Batch No.:L87-84	Henry's Law Constant (H) = 3.2×10^{-2} Pa m^3/mol	Acceptable. Calculation based on vapour pressure and solubility.	n/a	Study No.: 2017/1189884; Daum, A; 2017

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td>(99.0 %)</td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="7">B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)</td></tr>
<tr><td>Physical state and colour
B.2.3/01</td><td>Visual and olfactory inspection</td><td>BAS 684 H Batch No.:L87-84 (99.0 %)</td><td>Clear colourless liquid, faint fruity smell</td><td>Acceptable</td><td>Y</td><td>Study No.: 2015/1257674; Daum, A; 2015</td></tr>
<tr><td colspan="7">B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY</td></tr>
<tr><td>Ultraviolet/visible (UV/VIS)
B.2.4/01</td><td>OECD 101 UV-Visible Spectro-photometer</td><td>BAS 684 H Batch No.:L87-84 (99.0 %)</td><td>UV/VIS Spectrum in methanol (pH = 6.8)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>209</td><td>1.0315</td><td>8671.6</td></tr>
<tr><td>262</td><td>0.0320</td><td>269.0</td></tr>
<tr><td>290</td><td>-0.0002</td><td>-1.7</td></tr>
<tr><td>295</td><td>-0.0004</td><td>-3.4</td></tr>
<tr><td>320</td><td>-0.0002</td><td>-1.7</td></tr>
</table>
UV/VIS Spectrum in aqueous conditions (pH = 6.0)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>196</td><td>2.6256</td><td>22072.9</td></tr>
<tr><td>208</td><td>1.0437</td><td>8774.2</td></tr>
<tr><td>263</td><td>0.0390</td><td>327.9</td></tr>
<tr><td>290</td><td>0.0005</td><td>4.2</td></tr>
<tr><td>295</td><td>0.0002</td><td>1.7</td></tr>
<tr><td>320</td><td>0.0002</td><td>1.7</td></tr>
</table>
UV/VIS Spectrum in acidic conditions (pH = 1.4)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
</table></td><td>Acceptable

No absorption maxima were observed above 290 nm for each of the pH mediums, which indicates that the active substance has little or no potential to undergo photolytic degradation in the environment under acidic, basic or neutral conditions.</td><td>Y</td><td>Study No.: 2016/1051361; Daum, A; 2016</td></tr>
</table>

<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td>
<table>
<tr><td>199</td><td>1.4424</td><td>12125.9</td></tr>
<tr><td>208</td><td>1.0430</td><td>8768.3</td></tr>
<tr><td>263</td><td>0.0402</td><td>338.0</td></tr>
<tr><td>290</td><td>0.0004</td><td>3.4</td></tr>
<tr><td>295</td><td>0.0002</td><td>1.7</td></tr>
<tr><td>320</td><td>0.0002</td><td>1.7</td></tr>
</table>
UV/VIS Spectrum in basic conditions (pH = 12.1)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>215</td><td>0.7158</td><td>6017.6</td></tr>
<tr><td>263</td><td>0.0372</td><td>312.7</td></tr>
<tr><td>290</td><td>-0.0014</td><td>-11.8</td></tr>
<tr><td>295</td><td>-0.0015</td><td>-12.6</td></tr>
<tr><td>320</td><td>-0.0005</td><td>-4.2</td></tr>
</table>
</td><td></td><td></td><td></td></tr>
<tr><td>Infrared (IR)
B.2.4/02</td><td>ATR-FT IR spectrum obtained using Thermo Nicolet 6700 spectrometer</td><td>BAS 684 H Batch No.:L87-84 (99.0 %)</td><td>
ATR-FT IR between 550-4000 cm^{-1}
<table>
<tr><th>Wavenumber (cm^{-1})</th><th>Functional Group</th></tr>
<tr><td>741</td><td>C-H (aromatic stretching)</td></tr>
<tr><td>853</td><td>Cycloalkane(deformation)</td></tr>
<tr><td>882</td><td>Cycloalkane(deformation)</td></tr>
<tr><td>897</td><td>Cycloalkane (deformation)</td></tr>
<tr><td>1044</td><td>Aromatic (deformation) / Ar-CH$_3$</td></tr>
<tr><td>1067</td><td>C-O (ether stretching) / Ar-CH$_3$</td></tr>
<tr><td>1091</td><td>C-O (ether stretching)</td></tr>
<tr><td>1351</td><td>C-H (deformation)</td></tr>
<tr><td>1366</td><td>C-H (deformation)</td></tr>
<tr><td>1380</td><td>C-H (deformation)</td></tr>
<tr><td>1462</td><td>C-C (aromatic stretching)</td></tr>
<tr><td>2874</td><td>C-H (stretching)</td></tr>
<tr><td>2961</td><td>C-H (stretching)</td></tr>
</table>
</td><td>Acceptable

The suggested peak assignment is plausible. There are no unaccounted peaks or peaks which would be unlikely in a compound of this structure. Overall the spectrum is consistent with the structure.</td><td>Y</td><td>Study No.: 2016/1051361; Daum, A; 2016</td></tr>
</table>

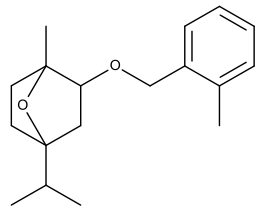
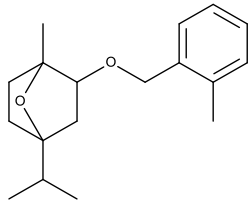
<table>
<tr><th>Test or Study Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr>
<td>Nuclear magnetic resonance (NMR)
B.2.4/03</td>
<td>Agilent 600 MHz NMR spectrometer</td>
<td>BAS 684 H Batch No.:L87-84 (99.0 %)</td>
<td>


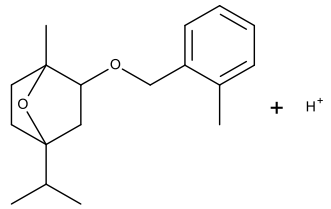
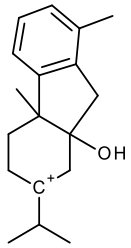
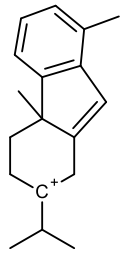
^{1}H-NMR (600 MHz, DMSO-d$_6$)
<table>
<tr><th>Atom</th><th>δH (ppm)</th><th>Rel. No. of H</th></tr>
<tr><td>17</td><td>0.91</td><td>6*</td></tr>
<tr><td>18</td><td>0.91</td><td>6*</td></tr>
<tr><td>20</td><td>1.34</td><td>3</td></tr>
<tr><td>15</td><td>1.41</td><td>6*</td></tr>
<tr><td>1</td><td>1.41</td><td>6*</td></tr>
<tr><td>13</td><td>1.45</td><td>6*</td></tr>
<tr><td>1</td><td>1.48</td><td>6*</td></tr>
<tr><td>13</td><td>1.93</td><td>3*</td></tr>
<tr><td>16</td><td>1.96</td><td>3*</td></tr>
<tr><td>8</td><td>2.26</td><td>3</td></tr>
<tr><td>3</td><td>3.59</td><td>1</td></tr>
<tr><td>5</td><td>4.30</td><td>1</td></tr>
<tr><td>5</td><td>4.44</td><td>1</td></tr>
<tr><td>9</td><td>7.15</td><td>3*</td></tr>
<tr><td>11</td><td>7.16</td><td>3*</td></tr>
<tr><td>10</td><td>7.18</td><td>3*</td></tr>
<tr><td>12</td><td>7.30</td><td>1</td></tr>
</table>
* indicates where signals overlap

^{13}C-NMR (150 MHz, DMSO-d$_6$)
<table>
<tr><th>Atom</th><th>δC (ppm)</th><th>Rel. No. of C</th></tr>
<tr><td>20</td><td>16.44</td><td>1</td></tr>
<tr><td>14</td><td>17.92</td><td>1</td></tr>
<tr><td>18</td><td>17.92</td><td>1</td></tr>
</table>
</td>
<td>Acceptable

^{1}H-NMR:
All expected peaks are accounted for. The dd observed at 3.59 ppm indicates the exo configuration of the bicyclic ring (the endo configuration would be characterised by an additional ^{4}J coupling between the 3H and 1-H, resulting in the splitting of this signal to a ddd). The spectrum is consistent with the expected structure.

^{13}C-NMR:
All carbons expected to be observed in the spectrum are assigned and the signal assignments considered appropriate. The spectrum is consistent with the expected structure.</td>
<td>Y</td>
<td>Study No.: 2016/1051361; Daum, A; 2016</td>
</tr>
</table>

<table>
<tr><th>Test or Study
Annex Point</th><th>Guideline
and method</th><th>Test material
purity and
specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td>
<table>
<tr><td>8</td><td>18.33</td><td>1</td></tr>
<tr><td>15</td><td>31.64</td><td>1</td></tr>
<tr><td>16</td><td>32.15</td><td>1</td></tr>
<tr><td>1</td><td>33.56</td><td>1</td></tr>
<tr><td>13</td><td>41.43</td><td>1</td></tr>
<tr><td>5</td><td>67.88</td><td>1</td></tr>
<tr><td>3</td><td>82.80</td><td>1</td></tr>
<tr><td>2</td><td>84.72</td><td>1</td></tr>
<tr><td>14</td><td>87.54</td><td>1</td></tr>
<tr><td>11</td><td>125.46</td><td>1</td></tr>
<tr><td>10</td><td>127.28</td><td>1</td></tr>
<tr><td>12</td><td>127.94</td><td>1</td></tr>
<tr><td>9</td><td>129.75</td><td>1</td></tr>
<tr><td>7</td><td>135.97</td><td>1</td></tr>
<tr><td>6</td><td>136.51</td><td>1</td></tr>
</table>
</td><td></td><td></td><td></td></tr>
<tr><td>Mass spectra (MS)
B.2.4/04</td><td>Thermo
QExactive</td><td>BAS 684 H
Batch
No.:L87-84
(99.0 %)</td><td>MS (ESI fullscan MS):
m/z = 297.18  + Na^+
m/z = 292.2  + NH_4^+</td><td>Acceptable
The obtained MS spectra are in agreement with the proposed structure.</td><td>Y</td><td>Study No.:
2016/1051361;
Daum, A; 2016</td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			m/z = 275.2  + H^+  m/z= 257  m/z= 239			

<table>
<tr><th>Test or Study
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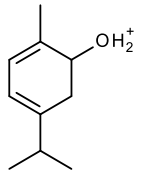
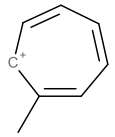
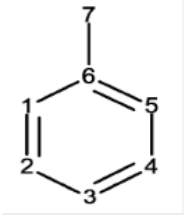
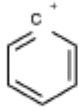
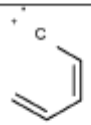
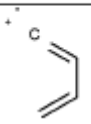
and method</th><th>Test material
purity and
specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td> 
m/z=153
 
m/z=105</td><td></td><td></td><td></td></tr>
<tr><td>Spectra for impurities
B.2.4/05</td><td>OECD 101
UV-Visible
Spectro-
photometer

ATR-FT IR
spectrum
obtained
using
Thermo
Nicolet
6700
spectrometer</td><td>Toluene
(BASF Reg.
No. 4005250)
Batch 1027B
(99.9 %)</td><td>UV/VIS Spectrum in methanol
<table><tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr><tr><td>207</td><td>1.1932</td><td>8062.4</td></tr><tr><td>290</td><td>0.0068</td><td>45.9</td></tr><tr><td>295</td><td>0.0051</td><td>34.5</td></tr><tr><td>320</td><td>0.0042</td><td>28.4</td></tr></table>
ATR-FT IR between 400-4000 cm^{-1}
<table><tr><th>Wavenumber (cm^{-1})</th><th>Functional Group</th></tr><tr><td>693</td><td>C-H (aromatic stretching)</td></tr><tr><td>726</td><td>C-H (aromatic stretching)</td></tr><tr><td>1458</td><td>C-C (aromatic stretching)</td></tr><tr><td>1495</td><td>C-C (aromatic stretching)</td></tr><tr><td>1604</td><td>C-C (aromatic stretching)</td></tr><tr><td>2947</td><td>C-H (aliphatic stretching)</td></tr><tr><td>3026</td><td>C-H (aliphatic stretching)</td></tr></table></td><td>Acceptable
The IR, NMR and MS spectra are in accordance with the impurity toluene.</td><td>Y</td><td>Study No.:
2017/1198003
Daum, A; 2017</td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	Agilent 600 MHz NMR spectrometer		 **^{1}H -NMR (600 MHz) ^{13}C-NMR (150 MHz), $CDCl_3$** Atom / δH (ppm) / δC (ppm) 1 / 7.25 / 129.09 2 / 7.32 / 128.28 3 / 7.23 / 125.35 4 / 7.32 / 128.28 5 / 7.25 / 129.09 6 / - / 137.90 7 / 2.42 / 21.49			
	MS (EI-TOF)		Structure / Formula / m/z Exp.  $C_6H_5^+$ 77.03960  $C_5H_6^+$ 66.04430  $C_4H_4^+$ 52.03057			

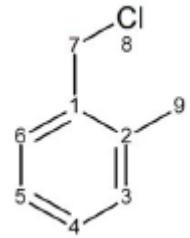
<table>
<tr><th>Test or Study
Annex Point</th><th>Guideline and method</th><th>Test material purity and specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr>
<td>Spectra for impurities
B.2.4/06</td>
<td>OECD 101
UV-Visible
Spectro-
photometer</td>
<td>2-
methylbenzyl
chloride
Batch No.:
02218MEV
(99.4%)</td>
<td>
UV/VIS Spectrum in methanol (pH = 6.9)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>201</td><td>0.8872</td><td>23371.0</td></tr>
<tr><td>217</td><td>0.2827</td><td>7447.0</td></tr>
<tr><td>290</td><td>-0.0001</td><td>-2.6</td></tr>
<tr><td>295</td><td>-0.0004</td><td>-10.5</td></tr>
<tr><td>320</td><td>0.0016</td><td>42.1</td></tr>
</table>
UV/VIS Spectrum in aqueous conditions (pH = 4.7)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>194</td><td>1.5577</td><td>41033.6</td></tr>
<tr><td>215</td><td>0.2749</td><td>7241.5</td></tr>
<tr><td>290</td><td>0.0010</td><td>26.3</td></tr>
<tr><td>295</td><td>0.0008</td><td>21.1</td></tr>
<tr><td>320</td><td>0.0016</td><td>42.1</td></tr>
</table>
UV/VIS Spectrum in acidic conditions (pH = 1.2)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>199</td><td>0.6875</td><td>18110.4</td></tr>
<tr><td>211</td><td>0.2950</td><td>7771.0</td></tr>
<tr><td>290</td><td>0.0005</td><td>13.2</td></tr>
<tr><td>295</td><td>0.0005</td><td>13.2</td></tr>
<tr><td>320</td><td>0.0011</td><td>29.0</td></tr>
</table>
UV/VIS Spectrum in basic conditions (pH = 12.3)
<table>
<tr><th>Wavelength (nm)</th><th>Absorbance (AU)</th><th>Molar Extinction Coefficient (L x mol^{-1} x cm^{-1})</th></tr>
<tr><td>217</td><td>0.1846</td><td>4862.8</td></tr>
<tr><td>290</td><td>-0.0009</td><td>-23.7</td></tr>
</table>
</td>
<td>Acceptable
The IR, NMR and MS spectra are in accordance with those expected for the impurity 2-methylbenzylchloride.</td>
<td>Y</td>
<td>Study No.:
2017/1156024
Daum, A; 2017</td>
</tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	ATR-FT IR spectrum obtained using Thermo Nicolet iS5 spectrometer Agilent 600 MHz NMR spectrometer					

295	-0.0011	-29.0
320	0.003	7.9

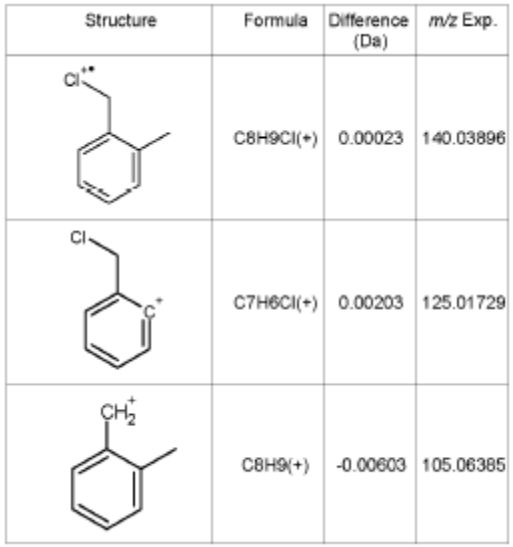
ATR-FT IR between 400-4000 cm^{-1}

Wavenumber (cm^{-1})	Functional Group
725	C-Cl (stretching vibration)
1461	CH_3 (deformation vibration)
2970	C-H (aliphatic stretching)

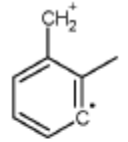
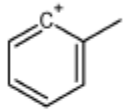
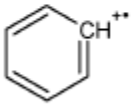
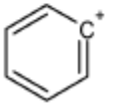


^{1}H -NMR (600 MHz) ^{13}C-NMR (150 MHz), $CDCl_3$

Atom	δH (ppm)	δC (ppm)
1	-	135.46
2	-	137.14
3	7.22	130.66
4	7.26	128.87
5	7.20	126.28
6	7.33	129.73
7	4.63	44.78
8	-	-
9	2.45	18.67

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	MS (GC-EI-TOF)					

Structure	Formula	Difference (Da)	*m/z* Exp.
	C8H9Cl(+)	0.00023	140.03896
	C7H6Cl(+)	0.00203	125.01729
	C8H9(+)	-0.00603	105.06385

<table>
<tr><th>Test or Study
Annex Point</th><th>Guideline
and method</th><th>Test material
purity and
specification</th><th>Used methods / Results</th><th>Comments (Acceptable / Non acceptable)</th><th>GLP</th><th>Reference</th></tr>
<tr><td></td><td></td><td></td><td>
<table>
<tr><td>  </td><td>C8H8(+)</td><td>0.00085</td><td>104.06290</td></tr>
<tr><td>  </td><td>C7H7(+)</td><td>0.00079</td><td>91.05502</td></tr>
<tr><td>  </td><td>C6H6(+)</td><td>0.00056</td><td>78.04696</td></tr>
<tr><td>  </td><td>C6H5(+)</td><td>0.00018</td><td>77.03876</td></tr>
</table>
</td><td></td><td></td><td></td></tr>
<tr><td colspan="7">B.2.5. SOLUBILITY IN WATER</td></tr>
<tr><td>Solubility in water
B.2.5/01</td><td>EEC A6
OECD 105
EPA
OCSPP
830.7840</td><td>BAS 684 H
Batch No.:
L2017-052
(98.9 %)</td><td>
<table>
<tr><th>Solvent</th><th>Solubility (g/L)</th><th>pH (measured)</th></tr>
<tr><td>deionised water</td><td>0.069</td><td>8.9</td></tr>
<tr><td>buffer pH 4</td><td>0.063</td><td>4.1</td></tr>
<tr><td>buffer pH 7</td><td>0.058</td><td>7.0</td></tr>
<tr><td>buffer pH 9</td><td>0.062</td><td>9.0</td></tr>
</table>
Results were obtained at 20 °C.
</td><td>Acceptable
The water solubility of BAS 684 H is low and is not significantly affected by pH.
Analysis of samples by HPLC-UV method (fully validated - see section B5.1.2.7).</td><td>Y</td><td>Study No.:
2017/1077867
Daum A; 2017</td></tr>
<tr><td colspan="7">B.2.6. SOLUBILITY IN ORGANIC SOLVENTS</td></tr>
<tr><td>Solubility in organic solvents
B.2.6/01</td><td>CIPAC MT
181</td><td>BAS 684 H
Batch No.:
COD-002038</td><td>
<table>
<tr><th>Solvent</th><th>Solubility (g/L)</th></tr>
<tr><td>n-heptane</td><td>>500</td></tr>
<tr><td>p-xylene</td><td>>500</td></tr>
<tr><td>1,2-dichloroethane</td><td>>500</td></tr>
</table>
</td><td>Acceptable
Analysis of n-heptane, p-xylene, 1,2-</td><td>Y</td><td>Study No.:
2017/1077869
Daum A; 2017</td></tr>
</table>

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
	Imaging analysis based on fluorescence contrast	(93.0 %) BAS 684 H Batch No.: COD-002038 (94.9 %)	methanol >500 acetone >500 ethyl acetate >500 Results were obtained at 25 °C. The two-photon excited fluorescence microscopy demonstrated that BAS 684 H preparations in DMSO in the concentration range of 12 - 430 mg/mL bear fluorescent droplets of increasing size. These droplets represent phase separated BAS 684 H in DMSO, since DMSO itself does not show any fluorescence in the detection channel. Therefore, it is concluded that BAS 684 H is not completely dissolved in DMSO down to concentrations of 12 mg/mL. In contrast, acetone is a better solvent for BAS 684 H. Up to 430 mg/mL BAS 684 H can be dissolved in acetone without any observable phase separation.	dichloroethane, methanol, acetone using shake flask method. BAS 684 H dissolved completely after addition of the solvents and is therefore considered to be readily soluble in all organic solvent (>500 g/L). This additional study confirmed that the solubility of BAS 684 H in acetone is >430 g/L. BAS 684 H was not soluble in DMSO at the lowest tested concentration of 12 g/L. This test was not performed under GLP, however the study was designed to test the best solvent for use in toxicology studies and is considered as supporting information only, therefore GLP is not necessary.	N	Study No.: 2018/1000729 Rückel, M; 2018
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER						
Partition coefficient n-octanol/water B.2.7/01	EC A8 OECD 117	BAS 684 H Batch No.:L87-84 (99.0 %)	Cinmethylin log P_{ow} = 4.5 at 20°C and pH=5.8 Estimated log P_{ow} = 4.63 (ADC/Labs software module)	Acceptable The measured log P_{ow} value confirms the estimated log P_{ow} of 4.63. As no dissociation occurs (see B.2.8/01 below), the pH dependency of the partition coefficient was not investigated. As log P_{ow} >4, the active substance has the potential to bioaccumulate.	Y	Study No.: 2016/1211635 Daum A; 2016
Partition coefficient n-octanol/water B.2.7/02 (metabolites)	EC A8 OECD 117	M684H005 (96.5 %) M684H006 (88.5 %)	M684H005 (BASF Reg. No. 6067256) Log P_{ow} = 2.3 at 20 °C and pH=6 M684H006 (BASF Reg. No. 6067258) Log Pow = 2.0 at 20 °C and pH=4 Log Pow = 0.6 at 20 °C and pH=7 Log Pow = 0.9 at 20 °C and pH=9	Acceptable The n-octanol/water partition coefficients were determined in the aqueous phase using HPLC-UV-DAD with calibration using reference values of known compounds. pH dependency of the partition coefficients was not investigated as no dissociation is expected based on the structure of the	Y	Study No.: 2017/1077875 Daum A; 2017 Study No.: 2017/1077876 Daum A; 2017

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
		M684H004 (97.8 %)	M684H004 (BASF Reg. No. 6055480) Log P_{ow} = 3.3 at 20 °C and pH=6	compounds, with the exception of M684H006 and M684H001. For M684H006 the log P_{ow} was determined in the aqueous phase (buffered solutions). In unbuffered aqueous solution no log P_{ow} could be determined as only a broad peak shape could be observed due to the dissociation in water. For M684H001 the log P_{ow} was determined in the aqueous phase and in buffered solutions.		Study No.: 2017/1077874 Daum A; 2017
		M684H002 (100 %)	M684H002 (Reg. No.6055479) Log P_{ow} = 3.0 at 20 °C and pH=6			Study No.: 2017/1077873 Daum A; 2017
		M684H001 (99.9 %)	M684H001 (BASF Reg. No. 6055521) Log P_{ow} =2.2 at 20 °C and pH=6 Log P_{ow} =2.9 at 20 °C and pH=4 Log P_{ow} =1.5 at 20 °C and pH=7 Log P_{ow} =1.6 at 20 °C and pH=9			Study No.: 2017/1077870 Daum A; 2017 Study No.: 2017/1077872 Daum A; 2017
		M684H003 (99.7 %)	M684H003 (BASF Reg. No. 4539586) Log P_{ow} =1.7 at 20 °C and pH=5.8			Study No.: 2018/1068463 Daum A; 2018
		M684H026 (98.2 %)	M684H026 (BASF Reg. No. 6059081) Log P_{ow} =0.8 at 20 °C and pH=5.8			
B.2.8. DISSOCIATION IN WATER						
Dissociation constant B.2.8/01	OECD 112	BAS 684 H Batch No.: L2017-052 (98.9 %)	No dissociation was observed for the test item in the range between pH 3.2 and pH 10.9.	Acceptable The active substance BAS 684 H does not dissociate in water and therefore no pKa value can be determined.	Y	Study No. 2017/1156023 Daum A; 2017
B.2.9. FLAMMABILITY AND SHELF-HEATING						
Flammability B.2.9/01	Waiver	BAS 684 H Batch No.: COD-002038 (93.0 %)	Based on the measured flash point of 156.5 °C the test item is not classified as a flammable liquid according to GHS or CLP Regulation EC 1272/2008.	Acceptable	Y	Study No.: 2017/1012634 Smeykal H; 2017

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
Self-heating B.2.9/02	EC A15	BAS 684 H Batch No.: COD-002038 (93.0 %)	The auto ignition temperature of the active substance is 375 °C atmospheric pressure.	Acceptable Cinmethylin is not classified as self-heating.	Y	Study No.: 2017/1012634 Smeykal H; 2017
B.2.10. FLASH POINT						
Flash point B.2.10/01	EC A9	BAS 684 H Batch No.: COD-002038 (93.0 %)	156.5 °C	Acceptable	Y	Study No.: 2017/1012634 Smeykal H; 2017
B.2.11. EXPLOSIVE PROPERTIES						
Explosive properties B.2.11/01	EC A14 OECD 113	BAS 684 H Batch No.: COD-002038 (93.0 %)	In the DSC measurement, the maximum energy of the exothermic decomposition of the test item cinmethylin was below the threshold of -500 J/g. Therefore, no further tests for explosive properties have to be performed. According to the results of the test on thermal stability, the test item does not have to be classified as explosive substance in class 1 according to the UN Transport Regulation.	Acceptable Cinmethylin is not classified as having explosive properties.	Y	Study No.: 2017/1012634 Smeykal H; 2017
B.2.12. SURFACE TENSION						
Surface tension B.2.12/01	EC A5 OECD 115	BAS 684 H Batch No.: L87-84 (99.0 %)	At 90 % of the saturation solubility in pure water: 50.3 mN/m.	Acceptable As cinmethylin has a surface tension below 60 mN/m it is surface active.	Y	Study No.: 2015/1257674; Daum, A; 2015
B.2.13. OXIDISING PROPERTIES						
Oxidizing properties B.2.13/01	EC A21	BAS 684 H Batch No.: COD-002038 (93.0 %)	The mean pressure rise time for cinmethylin is greater than the mean pressure rise time for the reference item nitric acid 65 %. Cinmethylin showed no oxidising properties according to Reg. (EC) No. 440/2008	Acceptable	Y	Study No.: 2017/1012634 Smeykal H; 2017

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			method A21. The test item does not have to be classified as oxidizing substance in division 5.1 according to the UN Transport Regulation.			
B.2.14. OTHER STUDIES						
Density **B.2.14/01**	EC A3 OECD 109	BAS 684 H Batch No.: L87-84 (99.0 %)	Density at 20 °C = 1.016 g/cm^3	Acceptable	Y	Study No.: 2015/1257674; Daum, A; 2015

Summary of physical and chemical properties of the active substance

Cinmethylin is a clear colorless liquid with faint fruity smell, with a boiling point of 330 °C (pure). Cinmethylin is not classified as flammable, explosive, or oxidising. The autoignition temperature of Cinmethylin technical material 375 °C with a flashpoint of 156.5 °C. The pure active substance is almost insoluble in pure water (0.058 g/L at pH 7.0), with no dissociation observed with the pH range 3.2 - 10.9 and a n-octanol/water partition coefficient log P_{OW} of 4.5 at 20 °C. UV/VIS, IR, NMR, and MS spectra are available for the active substance.

B.2.15. REFERENCES RELIED ON

Data Point	Author(s)	Year	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	Previous evaluation
KCA 2.1/01 KCA 2.1/02 KCA 2.1/03	Kroehl T	2019	Thermal Analysis of Cinmethylin (BAS 684 H, Reg. No. 900202) 2019/2054650 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.2/01 KCA 2.3/01 KCA 2.12/01 KCA 2.14/01	Daum A.	2015	Physical properties of Cinmethylin (BAS 684 H, Reg. No. 900202) - Pure active ingredient (PAI) 2015/1257674 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.2/02	Daum A	2017	Henry's law constant for Cinmethylin (BAS 684 H, Reg. No. 900202) 2017/1189884 BASF SE, Limburgerhof, Germany no Unpublished	N	N	Not applicable	BASF	None
KCA 2.4/01 KCA 2.4/02 KCA 2.4/03 KCA 2.4/04	Daum A.	2016	Mass, NMR, IR and UV/VIS spectra of Cinmethylin (Reg. No. 900202, BAS 684 H) PAI 2016/1051361 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.4/05	Daum A.	2017	Mass, NMR, IR and UV/VIS Spectrum of Toluene (Reg. No. 4005250) 2017/1198003 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.4/06	Daum A.	2017	Mass, NMR, IR and UV/VIS Spectrum of 2-Methylbenzylchlorid (Reg. No. 4262435) 2017/1156024 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None

Data Point	Author(s)	Year	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	Previous evaluation
KCA 2.5/01	Daum A.	2017	Water solubility of Cinmethylin (BAS 684 H) pure active ingredient (PAI) 2017/1077867 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.6/01	Daum A.	2017	Solubility of Cinmethylin (BAS 684 H) technical active ingredient (TGAI) in organic solvents 2017/1077869 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/01	Daum A.	2016	Partition coefficient n-Octanol/water (log Pow) of Cinmethylin (Reg. No. 900202, BAS 684 H) 2016/1211635 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6067256 (M684H005) 2017/1077875 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6067258 (M684H006) 2017/1077876 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6055480 (M684H004) 2017/1077874 BASF SE, Limburgerhof, Germany	N	Y	Data for first approval	BASF	None

Data Point	Author(s)	Year	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	Previous evaluation
			yes Unpublished					
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6055479 (M684H002) 2017/1077873 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6055521 (M684H001)) 2017/1077870 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2017	Partition coefficient n-octanol/water (log Pow) of Reg. No. 4539586 (M684H003) 2017/1077872 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.7/02	Daum A.	2018	Partition coefficient n-octanol/water (log Pow) of Reg. No. 6059081 (M684H026) 2018/1068463 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.8/01	Daum A.	2017	Dissociation constant (pKa) of Cinmethylin (BAS 684 H, Reg. No. 900202) PAI 2017/1156023 BASF SE, Limburgerhof, Germany yes Unpublished	N	Y	Data for first approval	BASF	None
KCA 2.9/01	Smeykal H.	2017	BAS 684 H (Cinmethylin) - Determination of physico-	N	Y	Data for first	BASF	None

Data Point	Author(s)	Year	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	Previous evaluation
KCA 2.10/01 KCA 2.11/01 KCA 2.13/01			chemical properties according to UN-Transport regulation and Directive 94/37/EC (Regulation (EC) No. 440/2008) 2017/1012634 consilab Gesellschaft fuer Anlagensicherheit mbH, Frankfurt/Main, Germany yes Unpublished			approval		