

Substance Name: 2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one

EC Number: 400-600-6

**CAS Number: 71868-10-5** 

# SUPPORT DOCUMENT FOR IDENTIFICATION OF

2-METHYL-1-(4-METHYLTHIOPHENYL)-2-MORPHOLINOPROPAN-1-ONE

AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS TOXIC FOR REPRODUCTION (ARTICLE 57C) PROPERTIES

# **CONTENTS**

IDENTIFICATION OF A SUBSTANCE OF VERY HIGH CONCERN ON THE THE CRITERIA SET OUT IN REACH ARTICLE 57	
JUSTIFICATION	5
1. IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PRO	PERTIES5
1.1 Name and other identifiers of the substance	5
2. HARMONISED CLASSIFICATION AND LABELLING	7
3. ENVIRONMENTAL FATE PROPERTIES	8
4. HUMAN HEALTH HAZARD ASSESSMENT	8
5. ENVIRONMENTAL HAZARD ASSESSMENT	8
6. CONCLUSIONS ON THE SVHC PROPERTIES	8
6.1 CMR assessment	8
REFERENCES	9

# **TABLES**

Table 1:	Substance identity	5
	Overview of physicochemical properties	
Table 3:	Classification according to Annex VI, Table 3.1 (list of harmonised	
	classification and labelling of hazardous substances) of Regulation	
	(EC) No 1272/2008	7

# IDENTIFICATION OF A SUBSTANCE OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57

**Substance name:** 2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one

**EC number:** 400-600-6

**CAS number:** 71868-10-5

The substance is identified as a substance meeting the criteria of Article 57 (c) of Regulation (EC) No 1907/2006 (REACH) owing to its classification in the hazard class toxic for reproduction category 1B<sup>1</sup>.

# Summary of how the substance meets the criteria set out in Article 57 of the REACH Regulation

2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one is covered by index number 606-041-00-6 of Regulation (EC) No 1272/2008 in Annex VI, part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances) and it is classified in the hazard class toxic for reproduction category 1B (H360FD: May damage fertility. May damage the unborn child.).

Therefore, this classification of the substance in Regulation (EC) No 1272/2008 shows that it meets the criteria for classification in the hazard class:

• Toxic for reproduction category 1B in accordance with Article 57 (c) of REACH.

Registration dossiers submitted for the substance: Yes

<sup>&</sup>lt;sup>1</sup> Classification in accordance with section 3.7. of Annex I to Regulation (EC) No 1272/2008.

# **Justification**

# 1. Identity of the substance and physical and chemical properties

# 1.1 Name and other identifiers of the substance

#### **Table 1: Substance identity**

EC number:	400-600-6
EC name:	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one
CAS number (in the EC inventory):	71868-10-5
CAS number: Deleted CAS numbers:	
CAS name:	
IUPAC name:	2-methyl-1-[4-(methylsulfanyl)phenyl]-2-(morpholin-4-yl)propan-1-one
Index number in Annex VI of the CLP Regulation	606-041-00-6
Molecular formula:	C15H21NO2S
Molecular weight range:	279.4
Synonyms:	Omnirad 907
	Irgacure 907
	Speedcure 97
	GENOCURE*PMP
	UV 907
	IHT-PI 907

#### Structural formula:

(source: European Chemicals Agency, <a href="http://echa.europa.eu/">http://echa.europa.eu/</a>)

# 1.2 Composition of the substance

Name: 2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one

**Description:** solid (particulate/powder)

**Substance type:** mono-constituent

There are no impurities relevant for the identification of the substance as a substance of very high concern (SVHC).

# 1.3 Physicochemical properties

**Table 2: Overview of physicochemical properties** 

Property	Description of key information	Value [Unit]	Reference/source of information	
Physical state at 20°C and 101.3 kPa	White to light beige powder	Solid	ECHA dissemination site: 07.05.2019	
Melting/freezing point	Measured, using photocell detection	74.6°C*	ECHA dissemination site: 07.05.2019	
Boiling point	Decomposed before boiling (decomposition at >190°C)	Not applicable	ECHA dissemination site: 07.05.2019	
Vapour pressure	Extrapolated value measurement by thermogravimetry (diffusion controlled evaporation)	0.0002 Pa at 25 °C	ECHA dissemination site: 07.05.2019	
Density	Measured by the air comparison pycnometer method	1210 kg/m³ at 33 °C	ECHA dissemination site: 07.05.2019	
Water solubility	Vater solubility Flask method		ECHA dissemination site: 07.05.2019	
Partition coefficient n- octanol/water (log value)	Shake flask method	3.09 at 25°C at pH 7	ECHA dissemination site: 07.05.2019	

<sup>\*</sup>QSAR-model MPBPVP v1.43 (Episuite v4.11) predicts a melting point of 133.12°C based on the chemical structure of the substance.

\*\*QSAR-model WSKOW v1.42 (Episuite v4.11) predicts a water solubility of 772.4 mg/L based on the

chemical structure of the substance.

# 2. Harmonised classification and labelling

2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one is covered by Index number 606-041-00-6 in part 3 of Annex VI to the CLP Regulation ( $10^{th}$  ATP) as follows:

Table 3: Classification according to Annex VI, Table 3.1 (list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008

Index No	Chemical Name	EC No	CAS No	Classification		Labelling			Spec.	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram, Signal Word Code(s)	Hazard statement code(s)	Suppl. Hazard statement code(s)	Conc. Limits, M- factors	
041- 00-6	methylthiopheny		68- 1 0-5	Repr. 1B Acute Tox. 4 * Aquatic Chronic 2	H360FD H302 H411	GHS08 GHS07 GHS09 Dgr	H360FD H302 H411			

# 3. Environmental fate properties

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c) of the REACH Regulation.

# 4. Human health hazard assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c) of the REACH Regulation.

### 5. Environmental hazard assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c) of the REACH Regulation.

# 6. Conclusions on the SVHC Properties

#### 6.1 CMR assessment

2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one is covered by index number 606-041-00-6 of Regulation (EC) No 1272/2008 in Annex VI, part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances) and it is classified in the hazard class toxic for reproduction category 1B (H360FD: May damage fertility. May damage the unborn child.).

Therefore, this classification of the substance in Regulation (EC) No 1272/2008 shows that it meets the criteria for classification in the hazard class:

• Toxic for reproduction category 1B in accordance with Article 57 (c) of REACH.

#### 6.2 PBT and vPvB assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c) of the REACH Regulation.

# **6.3 Assessment under Article 57(f)**

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c) of the REACH Regulation.

### **REFERENCES**

- EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC. Official Journal of the European Union, L396: 1-849.
- EU (2008). Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packing of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006. Official Journal of the European Union, L353: 1-1355.