

**Substance Name: 2-benzyl-2-dimethylamino-4'-  
morpholinobutyrophenone**

**EC Number: 404-360-3**

**CAS Number: 119313-12-1**

**SUPPORT DOCUMENT FOR IDENTIFICATION OF**

**2-BENZYL-2-DIMETHYLAMINO-4'-  
MORPHOLINOBTYROPHENONE**

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

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

**Substance name:** 2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone

**EC number:** 404-360-3

**CAS number:** 119313-12-1

- 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-benzyl-2-dimethylamino-4'-morpholinobutyrophenone is covered by index number 606-047-00-9 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 (H360D: 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**

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

## Justification

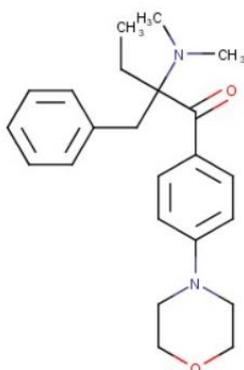
### 1. Identity of the substance and physical and chemical properties

#### 1.1 Name and other identifiers of the substance

**Table 1: Substance identity**

<b>EC number:</b>	404-360-3
<b>EC name:</b>	2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone
<b>CAS number (in the EC inventory):</b>	119313-12-1
<b>CAS number:</b> <b>Deleted CAS numbers:</b>	119313-12-1
<b>CAS name:</b>	1-butanone, 2-(dimethylamino)-1-[4-(4-morpholinyl)phenyl]-2-(phenylmethyl)-
<b>IUPAC name:</b>	2-benzyl-2-(dimethylamino)-1-[4-(morpholin-4-yl)phenyl]butan-1-one
<b>Index number in Annex VI of the CLP Regulation</b>	606-047-00-9
<b>Molecular formula:</b>	C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
<b>Molecular weight range:</b>	ca. 366.5
<b>Synonyms:</b>	Omnirad 369, Genocure BDMM, CG 25-369; IRGACURE 369; TK 11-319, Speedcure BDMM, Photoinitiator-369, Doublecure 369, Chivacure 169

#### Structural formula:



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

## 1.2 Composition of the substance

**Name:** 2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone

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

**Substance type:** multi-constituent

The substance includes a stereocentre and is regarded as a multi-constituent substance including the two main constituents:

(2S)-2-benzyl-2-(dimethylamino)-1-[4-(morpholin-4-yl)phenyl]butan-1-one and  
(2R)-2-benzyl-2-(dimethylamino)-1-[4-(morpholin-4-yl)phenyl]butan-1-one

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
<b>Physical state at 20°C and 101.3 kPa</b>	Slightly yellowish powder	Solid	ECHA dissemination site: 02.07.2019
<b>Melting/freezing point</b>	Capillary method	113.2 °C <sup>a</sup>	ECHA dissemination site: 02.07.2019
<b>Boiling point</b>	Decomposed at >275°C before boiling	Not applicable <sup>b</sup>	ECHA dissemination site: 02.07.2019
<b>Vapour pressure</b>	Extrapolated based on thermogravimetry (Diffusion controlled evaporation)	≤0.0000006 Pa at 25°C <sup>c</sup>	ECHA dissemination site: 02.07.2019
<b>Density</b>	Air comparison pycnometer method using Helium > 99.8 % as test gas	1210 kg/m <sup>3</sup> at 20°C	ECHA dissemination site: 02.07.2019
<b>Water solubility</b>	Flask method	5.9 mg/L at 20°C <sup>d</sup>	ECHA dissemination site: 02.07.2019
<b>Partition coefficient n-octanol/water (log value)</b>	Shake-flask method	2.91 at 25°C <sup>e</sup>	ECHA dissemination site: 02.07.2019

(a) QSAR-model MPBPWIN (v1.44) predicts a melting point of 190°C (weighted value)

(b) QSAR-model MPBPWIN (v1.44) predicts a melting point of 457°C

(c) QSAR-model MPBPWIN (v1.44): Selected VP: 7.97x10<sup>-7</sup> Pa (Modified Grain Method)

(d) QSAR-model WSKOW (v1.42) predicts a water solubility of 7.163 mg/L

(e) QSAR-model KOWWIN (v1.69) predicts a logPow of 4.50

## 2. Harmonised classification and labelling

2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone is covered by Index number 606-047-00-9 in part 3 of Annex VI to the CLP Regulation (13<sup>th</sup> 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. Conc. Limits, M-factors	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)		
606-047-00-9	2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone	404-360-3	119313-12-1	Repr. 1B Aquatic Acute 1 Aquatic Chronic 1	H360D H400 H410	GHS09 GHS08 Dgr	H360D H410			

### **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-benzyl-2-dimethylamino-4'-morpholinobutyrophenone is covered by index number 606-047-00-9 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 (H360D: 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.