SAFETY DATA SHEET
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier
Product name 2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol
Product number ID57870
Synonyms; trade names 11-(4-(2-Hydroxyethyl)-1-piperazinyl)dibenzo[b,f][1,4]thiazepine, Quetiapine impurity I, Quetiapine hydroxy impurity, DTHEP
CAS number 329216-67-3
EC number 700-085-0

1.2. Relevant identified uses of the substance or mixture and uses advised against
Identified uses Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet
Supplier Carbosynth Ltd
8&9 Old Station Business Park
Compton
Berkshire
RG20 6NE
UK
+44 1635 578444
+44 1635 579444
info@carbosynth.com

1.4. Emergency telephone number
Emergency telephone +44 7887 998634

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture
Classification (EC 1272/2008)
Physical hazards Not Classified
Health hazards Not Classified
Environmental hazards Not Classified

2.2. Label elements
EC number 700-085-0
Hazard statements NC Not Classified

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

3.1. Substances

<table>
<thead>
<tr>
<th>Product name</th>
<th>2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS number</td>
<td>329216-67-3</td>
</tr>
<tr>
<td>EC number</td>
<td>700-085-0</td>
</tr>
<tr>
<td>Chemical formula</td>
<td>C₁₉H₂₁N₃OS</td>
</tr>
</tbody>
</table>

SECTION 4: First aid measures

4.1. Description of first aid measures

**General information**
Get medical advice/attention if you feel unwell.

**Inhalation**
Remove person to fresh air and keep comfortable for breathing. If breathing stops, provide artificial respiration. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention if symptoms are severe or persist.

**Ingestion**
Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.

**Skin contact**
Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.

**Eye contact**
Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed

**General information**
See Section 11 for additional information on health hazards.

4.3. Indication of any immediate medical attention and special treatment needed

**Notes for the doctor**
Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

**Suitable extinguishing media**
Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

5.2. Special hazards arising from the substance or mixture

**Specific hazards**
None known.

**Hazardous combustion products**
Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon. Oxides of nitrogen. Oxides of sulphur.

5.3. Advice for firefighters

**Special protective equipment for firefighters**
Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

**Personal precautions**
Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust and vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage.

**6.2. Environmental precautions**
Environmental precautions
Avoid discharge into drains or watercourses or onto the ground.

**6.3. Methods and material for containment and cleaning up**
Methods for cleaning up
Wear protective clothing as described in Section 8 of this safety data sheet. Collect powder using special dust vacuum cleaner with particle filter or carefully sweep into suitable waste disposal containers and seal securely. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

**6.4. Reference to other sections**
Reference to other sections
For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

**SECTION 7: Handling and storage**

**7.1. Precautions for safe handling**
Usage precautions
Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid generation and spreading of dust. Avoid contact with skin and eyes. Avoid inhalation of dust and vapours.

**7.2. Conditions for safe storage, including any incompatibilities**
Storage precautions
Keep container tightly closed. Store in a cool and well-ventilated place. Store at temperatures between -15°C and -25°C.

**7.3. Specific end use(s)**
Specific end use(s)
The identified uses for this product are detailed in Section 1.2.

**SECTION 8: Exposure controls/Personal protection**

**8.1. Control parameters**
Occupational exposure limits
No exposure limits known for ingredient(s).

**8.2. Exposure controls**
Appropriate engineering controls
Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection
Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Hand protection
Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

Other skin and body protection
Wear appropriate clothing to prevent repeated or prolonged skin contact.
2-((4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

**Respiratory protection**  
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Particulate filters should comply with European Standard EN143. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

**Environmental exposure controls**  
Keep container tightly sealed when not in use.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Appearance</strong></td>
<td>Solid.</td>
</tr>
<tr>
<td><strong>Colour</strong></td>
<td>White. to Off-white. to Yellow.</td>
</tr>
<tr>
<td><strong>Odour</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Odour threshold</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>pH</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Melting point</strong></td>
<td>&gt;50°C</td>
</tr>
<tr>
<td><strong>Initial boiling point and range</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Flash point</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Evaporation rate</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Flammability (solid, gas)</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Upper/lower flammability or explosive limits</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Vapour pressure</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Vapour density</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Relative density</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Solubility(ies)</strong></td>
<td>Almost insoluble in the following materials: Chloroform. Ethanol. Methanol.</td>
</tr>
<tr>
<td><strong>Partition coefficient</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Auto-ignition temperature</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Decomposition Temperature</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Viscosity</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Explosive properties</strong></td>
<td>No data available.</td>
</tr>
<tr>
<td><strong>Oxidising properties</strong></td>
<td>No data available.</td>
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</table>

#### 9.2. Other information

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Molecular weight</strong></td>
<td>339.46</td>
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</table>

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactivity</strong></td>
<td>No data available.</td>
</tr>
</tbody>
</table>

#### 10.2. Chemical stability
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

Stability
Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions
Possibility of hazardous reactions
No data available.

10.4. Conditions to avoid
Conditions to avoid
No data available.

10.5. Incompatible materials
Materials to avoid
Strong oxidising agents.

10.6. Hazardous decomposition products
Hazardous decomposition products

SECTION 11: Toxicological information

11.1. Information on toxicological effects
Toxicological effects
Not regarded as a health hazard under current legislation.

Acute toxicity - oral
Notes (oral LD₅₀)
Based on available data the classification criteria are not met.

Acute toxicity - dermal
Notes (dermal LD₅₀)
Based on available data the classification criteria are not met.

Acute toxicity - inhalation
Notes (inhalation LC₅₀)
Based on available data the classification criteria are not met.

Skin corrosion/irritation
Animal data
Based on available data the classification criteria are not met.

Serious eye damage/irritation
Based on available data the classification criteria are not met.

Respiratory sensitisation
Based on available data the classification criteria are not met.

Skin sensitisation
Based on available data the classification criteria are not met.

Germ cell mutagenicity
Genotoxicity - in vitro
Based on available data the classification criteria are not met.

Carcinogenicity
Carcinogenicity
None of the ingredients are listed or exempt.

Reproductive toxicity
Reproductive toxicity - fertility
Based on available data the classification criteria are not met.

Reproductive toxicity - development
Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure
STOT - single exposure
Not classified as a specific target organ toxicant after a single exposure.
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

Specific target organ toxicity - repeated exposure
STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.
Aspiration hazard Not relevant. Solid.

General information No specific health hazards known. Dust may irritate the eyes and the respiratory system. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation Dust may irritate the respiratory system. Frequent inhalation of dust over a long period of time increases the risk of developing lung diseases.
Ingestion No specific symptoms known. May cause discomfort if swallowed.
Skin contact Prolonged contact may cause dryness of the skin.
Eye contact Dust may cause slight irritation.
Route of exposure Ingestion Inhalation Skin and/or eye contact
Target organs No specific target organs known.
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

SECTION 12: Ecological information

Ecotoxicity
Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity
Toxicity
Based on available data the classification criteria are not met.

12.2. Persistence and degradability
Persistence and degradability
The degradability of the product is not known.

12.3. Bioaccumulative potential
Bioaccumulative potential
No data available on bioaccumulation.

Partition coefficient
No data available.

12.4. Mobility in soil
Mobility
No data available.

12.5. Results of PBT and vPvB assessment
Results of PBT and vPvB assessment
No data available.

12.6. Other adverse effects
Other adverse effects
None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods
General information
Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

SECTION 14: Transport information

14.1. UN number
Not applicable.

14.2. UN proper shipping name
Not applicable.

14.3. Transport hazard class(es)
No transport warning sign required.

14.4. Packing group
Not applicable.

14.5. Environmental hazards
Environmentally hazardous substance/marine pollutant
No.

14.6. Special precautions for user
2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-piperazin-1-yl)-ethanol

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations
Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.

EU legislation

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet
ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
IATA: International Air Transport Association.
IMDG: International Maritime Dangerous Goods.
CAS: Chemical Abstracts Service.
ATE: Acute Toxicity Estimate.
LC₅₀: Lethal Concentration to 50 % of a test population.
LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).
EC₅₀: 50% of maximal Effective Concentration.
PBT: Persistent, Bioaccumulative and Toxic substance.
vPvB: Very Persistent and Very Bioaccumulative.

Training advice
Only trained personnel should use this material.

Revision date
20/02/2020

Revision
1

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.