

Melting Point Standard Set Vanillin (81-83 °C), Phenacetin (134-136 °C), Caffeine (235-237 °C)

Product No.	85113
Version	7.0
Revision date	30.12.2017
Print date	30.12.2017

Composition / Information on ingredients

85113-1	Melting Point Standard Vanillin 81 to 83 °C
85113-2	Melting Point Standard Phenacetin 133 to 135 °C
85113-3	Melting Point Standard Caffeine 235 to 238 °C

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)

Revision date: 30.12.2017

Version: 7.0

Print date: 30.12.2017

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

1.1 Product identifier

Trade name/designation:	Melting Point Standard Vanillin 81 to 83 °C
Product No.:	85113-1
CAS No.:	121-33-5
INDEX No.:	000-000-00-0
REACH No.:	Not yet communicated down the supply chain.
Other means of identification:	no data available

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	General chemical reagent
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1.3 Details of the supplier of the safety data sheet

United Kingdom

VWR International Ltd.

Street	Hunter Boulevard, Magna Park
Postal code/city	Lutterworth, LE17 4XN
Telephone	0800 22 33 44
Telefax	01455 55 85 86
E-mail (competent person)	SDS@vwr.com

Emergency telephone

Telephone	+44 (0) 1270 502894 (CareChem24)
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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

2.1.1 Classification according to Regulation (EC) No. 1272/2008 [CLP]

Hazard classes and hazard categories	Hazard statements
Eye irritation, category 2	H319

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms



Signal word: Warning

Hazard statements	
H319	Causes serious eye irritation.

Precautionary statements	
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Other hazards

none

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name	Vanillin
Molecular formula	C ₈ H ₈ O ₃
Molecular weight	152.15 g/mol
CAS No.	121-33-5
REACH registration No.	Not yet communicated down the supply chain.
INDEX No.	000-000-00-0



SECTION 4: First aid measures

4.1 General information

If exposed or if you feel unwell: Call a POISON CENTRE or doctor/physician. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

After inhalation

Call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

In case of ingestion

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do NOT induce vomiting. Give nothing to eat or drink.

4.2 Most important symptoms and effects, both acute and delayed

no data available

4.3 Indication of any immediate medical attention and special treatment needed

no data available

4.4 Self-protection of the first aider

First aider: Pay attention to self-protection!

4.5 Information to physician

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

The product itself does not burn.
Co-ordinate fire-fighting measures to the fire surroundings.

Extinguishing media which must not be used for safety reasons

no restriction

5.2 Special hazards arising from the substance or mixture

In case of fire may be liberated:
Carbon monoxide
Carbon dioxide (CO₂)

5.3 Advice for firefighters

DO NOT fight fire when fire reaches explosives.
Special protective equipment for firefighters
Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Do not allow run-off from fire-fighting to enter drains or water courses.

Do not inhale explosion and combustion gases.

Use water spray jet to protect personnel and to cool endangered containers.

In case of fire: Evacuate area.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid generation of dust.

6.2 Environmental precautions

Do not allow to enter into surface water or drains.

6.3 Methods and material for containment and cleaning up

Spilled product must never be returned to the original container for recycling. Clean contaminated objects and areas thoroughly observing environmental regulations. Collect in closed and suitable containers for disposal.

6.4 Additional information

Clear spills immediately.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

All work processes must always be designed so that the following is as low as possible: Inhalation skin contact Eye contact If handled uncovered, arrangements with local exhaust ventilation have to be used. If local exhaust ventilation is not possible or not sufficient, the entire working area must be ventilated by technical means. Usual measures for fire prevention. Handle under (Gas): Protective gas, dry

7.2 Conditions for safe storage, including any incompatibilities

Recommended storage temperature: 15-25°C

Storage class: 10-13

Keep container tightly closed and in a well-ventilated place. Store product under (gas): Protective gas, dry Do not allow contact with air.

7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Does not contain substances above concentration limits fixing an occupational exposure limit.

8.2 Exposure controls

8.2.1 Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment. If handled uncovered, arrangements with local exhaust ventilation have to be used.

8.2.2 Personal protection equipment

Wear suitable protective clothing. When handling with chemical substances, protective clothing with CE-labels including the four control digits must be worn.

Eye/face protection

Eye glasses with side protection DIN-/EN-Norms: DIN EN 166

Recommendation: VWR 111-0432

Skin protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. Recommended glove articles DIN-/EN-Norms: DIN EN 374 In the case of wanting to use the gloves again, clean them before taking off and air them well.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-0998

By long-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,38 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-3717 / 112-1381

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Suitable respiratory protection apparatus:	Filtering Half-face mask (DIN EN 149)
Recommendation:	VWR 111-0451
Suitable material:	P3
Recommendation:	VWR 111-0244

Additional information

Wash hands before breaks and after work. Avoid contact with skin and eyes. When using do not eat, drink or smoke. Provide eye shower and label its location conspicuously.

8.2.3 Environmental exposure controls

no data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

(a) Appearance	
Physical state:	solid
Colour:	cream
(b) Odour:	no data available
(c) Odour threshold:	no data available

Safety relevant basic data

(d) pH:	4-5 (10 g/l; H ₂ O; 20 °C)
(e) Melting point/freezing point:	~ 82 °C
(f) Initial boiling point and boiling range:	285 °C (1013 hPa)
(g) Flash point:	153 °C
(h) Evaporation rate:	no data available
(i) Flammability (solid, gas):	not applicable
(j) Flammability or explosive limits	
Lower explosion limit:	no data available
Upper explosion limit:	no data available
(k) Vapour pressure:	0.0029 hPa (25 °C)
(l) Vapour density:	no data available
(m) Relative density:	1.056 g/cm ³ (20 °C)
(n) Solubility(ies)	
Water solubility (g/L):	10 g/l (25 °C)
Soluble (g/L) in Ethanol:	no data available
(o) Partition coefficient: n-octanol/water:	1.37 (20 °C)
(p) Auto-ignition temperature:	> 400 °C
(q) Decomposition temperature:	no data available
(r) Viscosity	
Kinematic viscosity:	no data available
Dynamic viscosity:	no data available
(s) Explosive properties:	not applicable
(t) Oxidising properties:	not applicable

9.2 Other information

Bulk density:	1.056 g/cm ³ (20 °C)
Refraction index:	1.555 (589 nm; 25 °C)
Dissociation constant:	no data available
Surface tension:	no data available
Henry constant:	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

10.7 Additional information

no data available

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute effects

Acute oral toxicity:

LD50: > 4200 mg/kg - Rat - (OECD 401)

Acute dermal toxicity:

LD50: < 5010 mg/kg - Rabbit - (IUCLID)

Acute inhalation toxicity:

no data available

Irritant and corrosive effects

Primary irritation to the skin:

not applicable

Irritation to eyes:

Causes serious eye irritation.

Irritation to respiratory tract:

not applicable

Respiratory or skin sensitisation

In case of skin contact: not sensitising

After inhalation: not sensitising

STOT-single exposure

not applicable

STOT-repeated exposure

not applicable

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)

Carcinogenicity

No indication of human carcinogenicity.

Germ cell mutagenicity

No indications of human germ cell mutagenicity exist.

Reproductive toxicity

No indications of human reproductive toxicity exist.

Aspiration hazard

not applicable

Other adverse effects

no data available

Additional information

no data available

SECTION 12: Ecological information

12.1 Ecotoxicity

Fish toxicity:

no data available

Daphnia toxicity:

no data available

Algae toxicity:

no data available

Bacteria toxicity:

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water: 1.37 (20 °C)

12.4 Mobility in soil:

no data available

12.5 Results of PBT/vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal. Send to a hazardous waste incinerator facility under observation of official regulations.

Waste code product: no data available

Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

Additional information

no data available

SECTION 14: Transport information

Land transport (ADR/RID)

No dangerous good in sense of this transport regulation.

Sea transport (IMDG)

No dangerous good in sense of this transport regulation.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
not relevant

Air transport (ICAO-TI / IATA-DGR)

No dangerous good in sense of this transport regulation.



SECTION 15: Regulatory information

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

EU legislation

- 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 (Text with EEA relevance)
- Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance)
- Commission Regulation (EU) No 453/2010 of 20 May 2010 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (Text with EEA relevance)
- Commission Regulation (EU) 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

National regulations

no data available

Water hazard class (WGK):

slightly hazardous to water (WGK 1)

15.2 Chemical Safety Assessment

not relevant

SECTION 16: Other information

Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists

ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road

AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)

CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures

DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)

Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)

IATA-DGR - International Air Transport Association-Dangerous Goods Regulations

ICAO-TI - International Civil Aviation Organization-Technical Instructions

IMDG - International Maritime Code for Dangerous Goods

LTV - Long Term Value

NIOSH - National Institute for Occupational Safety and Health

OSHA - Occupational Safety & Health Administration

PBT - Persistent, Bioaccumulative and Toxic

RID - Regulation concerning the International Carriage of Dangerous Goods by Rail

STV - Short Term Value

SVHC - Substances of Very High Concern

vPvB - very Persistent, very Bioaccumulative

Additional information

Indication of changes: general update

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)

Revision date: 30.12.2017

Version: 7.0

Print date: 30.12.2017

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

1.1 Product identifier

Trade name/designation:	Melting Point Standard Phenacetin 133 to 135 °C
Product No.:	85113-2
CAS No.:	62-44-2
INDEX No.:	000-000-00-0
REACH No.:	Not yet communicated down the supply chain.
Other means of identification:	no data available

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	General chemical reagent
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1.3 Details of the supplier of the safety data sheet

United Kingdom

VWR International Ltd.

Street	Hunter Boulevard, Magna Park
Postal code/city	Lutterworth, LE17 4XN
Telephone	0800 22 33 44
Telefax	01455 55 85 86
E-mail (competent person)	SDS@vwr.com

Emergency telephone

Telephone	+44 (0) 1270 502894 (CareChem24)
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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

2.1.1 Classification according to Regulation (EC) No. 1272/2008 [CLP]

Hazard classes and hazard categories	Hazard statements
Carcinogenicity, category 1B	H350
Acute toxicity, category 4, oral	H302

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms



Signal word: Danger

Hazard statements	
H350	May cause cancer.
H302	Harmful if swallowed.

Precautionary statements	
P201	Obtain special instructions before use.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P301+P330+P331	IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P308+P313	IF exposed or concerned: Get medical advice/attention.

Other hazards

none

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name	4'-Ethoxyacetanilide
Molecular formula	C ₁₀ H ₁₃ NO ₂
Molecular weight	179.22 g/mol
CAS No.	62-44-2
REACH registration No.	Not yet communicated down the supply chain.
INDEX No.	000-000-00-0

SECTION 4: First aid measures

4.1 General information

If exposed or if you feel unwell: Call a POISON CENTRE or doctor/physician. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

After inhalation

Call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

In case of ingestion

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do NOT induce vomiting. Give nothing to eat or drink.

4.2 Most important symptoms and effects, both acute and delayed

no data available

4.3 Indication of any immediate medical attention and special treatment needed

no data available

4.4 Self-protection of the first aider

First aider: Pay attention to self-protection!

4.5 Information to physician

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

The product itself does not burn.
Co-ordinate fire-fighting measures to the fire surroundings.

Extinguishing media which must not be used for safety reasons

no restriction

5.2 Special hazards arising from the substance or mixture

In case of fire may be liberated:
Carbon monoxide
Carbon dioxide (CO₂)
Nitrogen oxides (NO_x)

5.3 Advice for firefighters

DO NOT fight fire when fire reaches explosives.
Special protective equipment for firefighters
Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Do not allow run-off from fire-fighting to enter drains or water courses.

Do not inhale explosion and combustion gases.

Use water spray jet to protect personnel and to cool endangered containers.

In case of fire: Evacuate area.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid generation of dust.

6.2 Environmental precautions

Do not allow to enter into surface water or drains.

6.3 Methods and material for containment and cleaning up

Spilled product must never be returned to the original container for recycling. Clean contaminated objects and areas thoroughly observing environmental regulations. Collect in closed and suitable containers for disposal.

6.4 Additional information

Clear spills immediately.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

All work processes must always be designed so that the following is as low as possible: Inhalation skin contact Eye contact

7.2 Conditions for safe storage, including any incompatibilities

Recommended storage temperature: no data available

Storage class: no data available

Keep container tightly closed and in a well-ventilated place.

7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Does not contain substances above concentration limits fixing an occupational exposure limit.

8.2 Exposure controls

8.2.1 Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment. If handled uncovered, arrangements with local exhaust ventilation have to be used.

8.2.2 Personal protection equipment

Wear suitable protective clothing. When handling with chemical substances, protective clothing with CE-labels including the four control digits must be worn.

Eye/face protection

Eye glasses with side protection DIN-/EN-Norms: DIN EN 166

Recommendation: VWR 111-0432

Skin protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. Recommended glove articles DIN-/EN-Norms: DIN EN 374 In the case of wanting to use the gloves again, clean them before taking off and air them well.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	480 min
Recommended glove articles:	VWR 112-0998

By long-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	480 min
Recommended glove articles:	VWR 112-0998

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Suitable respiratory protection apparatus:	Filtering Half-face mask (DIN EN 149)
Recommendation:	VWR 111-0451
Suitable material:	P3
Recommendation:	VWR 111-0244

Additional information

Wash hands before breaks and after work. Avoid contact with skin and eyes. When using do not eat, drink or smoke. Provide eye shower and label its location conspicuously.

8.2.3 Environmental exposure controls

no data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

(a) Appearance	
Physical state:	solid
Colour:	white
(b) Odour:	no data available
(c) Odour threshold:	no data available

Safety relevant basic data

(d) pH:	no data available
(e) Melting point/freezing point:	no data available
(f) Initial boiling point and boiling range:	no data available
(g) Flash point:	no data available
(h) Evaporation rate:	no data available
(i) Flammability (solid, gas):	not applicable
(j) Flammability or explosive limits	
Lower explosion limit:	no data available
Upper explosion limit:	no data available
(k) Vapour pressure:	no data available
(l) Vapour density:	no data available
(m) Relative density:	no data available
(n) Solubility(ies)	
Water solubility (g/L):	no data available
Soluble (g/L) in Ethanol:	no data available
(o) Partition coefficient: n-octanol/water:	no data available
(p) Auto-ignition temperature:	no data available
(q) Decomposition temperature:	no data available
(r) Viscosity	
Kinematic viscosity:	no data available
Dynamic viscosity:	no data available
(s) Explosive properties:	not applicable
(t) Oxidising properties:	not applicable

9.2 Other information

Bulk density:	no data available
Refraction index:	no data available
Dissociation constant:	no data available
Surface tension:	no data available
Henry constant:	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

10.7 Additional information

no data available

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute effects

Acute oral toxicity:

LD50: 1650 mg/kg - Rat - (Japan GHS Basis for Classification Data)

Acute dermal toxicity:

no data available

Acute inhalation toxicity:

no data available

Irritant and corrosive effects

Primary irritation to the skin:

not applicable

Irritation to eyes:

not applicable

Irritation to respiratory tract:

not applicable

Respiratory or skin sensitisation

In case of skin contact: not sensitising

After inhalation: not sensitising

STOT-single exposure

not applicable

STOT-repeated exposure

not applicable

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)

Carcinogenicity

May cause cancer.

Germ cell mutagenicity

No indications of human germ cell mutagenicity exist.

Reproductive toxicity

No indications of human reproductive toxicity exist.

Aspiration hazard

not applicable

Other adverse effects

no data available

Additional information

no data available

SECTION 12: Ecological information

12.1 Ecotoxicity

Fish toxicity:

no data available

Daphnia toxicity:

no data available

Algae toxicity:

no data available

Bacteria toxicity:

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water: no data available

12.4 Mobility in soil:

no data available

12.5 Results of PBT/vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal.

Waste code product: no data available

Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

Additional information

no data available

SECTION 14: Transport information

Land transport (ADR/RID)

No dangerous good in sense of this transport regulation.

Sea transport (IMDG)

No dangerous good in sense of this transport regulation.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
not relevant

Air transport (ICAO-TI / IATA-DGR)

No dangerous good in sense of this transport regulation.



SECTION 15: Regulatory information

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

EU legislation

- 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 (Text with EEA relevance)
- Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance)
- Commission Regulation (EU) No 453/2010 of 20 May 2010 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (Text with EEA relevance)
- Commission Regulation (EU) 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

National regulations

no data available

Water hazard class (WGK):

no data available

15.2 Chemical Safety Assessment

no data available

SECTION 16: Other information

Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists

ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road

AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)

CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures

DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)

Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)

IATA-DGR - International Air Transport Association-Dangerous Goods Regulations

ICAO-TI - International Civil Aviation Organization-Technical Instructions

IMDG - International Maritime Code for Dangerous Goods

LTV - Long Term Value

NIOSH - National Institute for Occupational Safety and Health

OSHA - Occupational Safety & Health Administration

PBT - Persistent, Bioaccumulative and Toxic

RID - Regulation concerning the International Carriage of Dangerous Goods by Rail

STV - Short Term Value

SVHC - Substances of Very High Concern

vPvB - very Persistent, very Bioaccumulative

Additional information

Indication of changes: general update

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)

Revision date: 30.12.2017

Version: 7.0

Print date: 30.12.2017

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

1.1 Product identifier

Trade name/designation:	Melting Point Standard Caffeine 235 to 238 °C
Product No.:	85113-3
CAS No.:	58-08-2 (5743-12-4)
INDEX No.:	613-086-00-5
REACH No.:	Not yet communicated down the supply chain.
Other means of identification:	no data available

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	General chemical reagent
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1.3 Details of the supplier of the safety data sheet

United Kingdom

VWR International Ltd.

Street	Hunter Boulevard, Magna Park
Postal code/city	Lutterworth, LE17 4XN
Telephone	0800 22 33 44
Telefax	01455 55 85 86
E-mail (competent person)	SDS@vwr.com

Emergency telephone

Telephone	+44 (0) 1270 502894 (CareChem24)
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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

2.1.1 Classification according to Regulation (EC) No. 1272/2008 [CLP]

Hazard classes and hazard categories	Hazard statements
Acute toxicity, category 4, oral	H302

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms



Signal word: Warning

Hazard statements	
H302	Harmful if swallowed.

Precautionary statements	
P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor/.../if you feel unwell.

Other hazards

none

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name	Caffeine
Molecular formula	C ₈ H ₁₀ N ₄ O ₂
Molecular weight	194.19 g/mol
CAS No.	58-08-2
REACH registration No.	Not yet communicated down the supply chain.
INDEX No.	613-086-00-5

SECTION 4: First aid measures

4.1 General information

IF exposed or if you feel unwell: Call a POISON CENTRE or doctor/physician. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

After inhalation

Call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

In case of ingestion

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do NOT induce vomiting. Give nothing to eat or drink.

4.2 Most important symptoms and effects, both acute and delayed

no data available

4.3 Indication of any immediate medical attention and special treatment needed

no data available

4.4 Self-protection of the first aider

First aider: Pay attention to self-protection!

4.5 Information to physician

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

The product itself does not burn.
Co-ordinate fire-fighting measures to the fire surroundings.

Extinguishing media which must not be used for safety reasons

no restriction

5.2 Special hazards arising from the substance or mixture

In case of fire may be liberated:
Carbon monoxide
Carbon dioxide (CO₂)
Nitrogen oxides (NO_x)

5.3 Advice for firefighters

DO NOT fight fire when fire reaches explosives.
Special protective equipment for firefighters
Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Do not allow run-off from fire-fighting to enter drains or water courses.
Do not inhale explosion and combustion gases.
Use water spray jet to protect personnel and to cool endangered containers.

In case of fire: Evacuate area.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid generation of dust.

6.2 Environmental precautions

Do not allow to enter into surface water or drains.

6.3 Methods and material for containment and cleaning up

Spilled product must never be returned to the original container for recycling. Clean contaminated objects and areas thoroughly observing environmental regulations. Collect in closed and suitable containers for disposal.

6.4 Additional information

Clear spills immediately.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

All work processes must always be designed so that the following is as low as possible: Inhalation skin contact Eye contact If handled uncovered, arrangements with local exhaust ventilation have to be used. If local exhaust ventilation is not possible or not sufficient, the entire working area must be ventilated by technical means. Usual measures for fire prevention. Handle under (Gas): Protective gas, dry

7.2 Conditions for safe storage, including any incompatibilities

Recommended storage temperature: 15-25°C

Storage class: 10-13

Keep container tightly closed and in a well-ventilated place.

7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Does not contain substances above concentration limits fixing an occupational exposure limit.

8.2 Exposure controls

8.2.1 Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment. If handled uncovered, arrangements with local exhaust ventilation have to be used.

8.2.2 Personal protection equipment

Wear suitable protective clothing. When handling with chemical substances, protective clothing with CE-labels including the four control digits must be worn.

Eye/face protection

Eye glasses with side protection DIN-/EN-Norms: DIN EN 166

Recommendation: VWR 111-0432

Skin protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. Recommended glove articles DIN-/EN-Norms: DIN EN 374 In the case of wanting to use the gloves again, clean them before taking off and air them well.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-0998

By long-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,38 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-3717 / 112-1381

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Suitable respiratory protection apparatus:	Filtering Half-face mask (DIN EN 149)
Recommendation:	VWR 111-0451
Suitable material:	P3
Recommendation:	VWR 111-0244

Additional information

Wash hands before breaks and after work. Avoid contact with skin and eyes. When using do not eat, drink or smoke. Provide eye shower and label its location conspicuously.

8.2.3 *Environmental exposure controls*
no data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

(a) Appearance	
Physical state:	solid
Colour:	white
(b) Odour:	no data available
(c) Odour threshold:	no data available

Safety relevant basic data

(d) pH:	6 (10 g/l; H ₂ O; 20 °C)
(e) Melting point/freezing point:	235-239 °C
(f) Initial boiling point and boiling range:	no data available
(g) Flash point:	no data available
(h) Evaporation rate:	no data available
(i) Flammability (solid, gas):	not applicable
(j) Flammability or explosive limits	
Lower explosion limit:	no data available
Upper explosion limit:	no data available
(k) Vapour pressure:	~ 20 hPa (80 °C)
(l) Vapour density:	no data available
(m) Relative density:	1.23 g/cm ³ (19 °C)
(n) Solubility(ies)	
Water solubility (g/L):	~20 g/l (20 °C)
Soluble (g/L) in Ethanol:	no data available
(o) Partition coefficient: n-octanol/water:	-0.07 (20 °C)
(p) Auto-ignition temperature:	> 600 °C (DIN 51794)
(q) Decomposition temperature:	no data available
(r) Viscosity	
Kinematic viscosity:	no data available
Dynamic viscosity:	no data available
(s) Explosive properties:	not applicable
(t) Oxidising properties:	not applicable

9.2 Other information

Bulk density:	1.23 g/cm ³ (19 °C)
Refraction index:	1.494 (589 nm; 20 °C)
Dissociation constant:	no data available
Surface tension:	no data available
Henry constant:	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

10.7 Additional information

no data available

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute effects

Acute oral toxicity:

LD50: < 261 mg/kg - Rat - (Merck KGaA)

Acute dermal toxicity:

LD50: < 2000 mg/kg - Rat - (Merck KGaA)

Acute inhalation toxicity:

no data available

Irritant and corrosive effects

Primary irritation to the skin:

not applicable

Irritation to eyes:

not applicable

Irritation to respiratory tract:

not applicable

Respiratory or skin sensitisation

In case of skin contact: not sensitising

After inhalation: not sensitising

STOT-single exposure

not applicable

STOT-repeated exposure

not applicable

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)

Carcinogenicity

No indication of human carcinogenicity.

Germ cell mutagenicity

No indications of human germ cell mutagenicity exist.

Reproductive toxicity

No indications of human reproductive toxicity exist.

Aspiration hazard

not applicable

Other adverse effects

no data available

Additional information

no data available

SECTION 12: Ecological information

12.1 Ecotoxicity

Fish toxicity:

no data available

Daphnia toxicity:

no data available

Algae toxicity:

no data available

Bacteria toxicity:

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water: -0.07 (20 °C)

12.4 Mobility in soil:

no data available

12.5 Results of PBT/vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal. Send to a hazardous waste incinerator facility under observation of official regulations.

Waste code product: no data available

Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

Additional information

no data available

SECTION 14: Transport information

Land transport (ADR/RID)

14.1	UN-No.:	1544
14.2	Proper Shipping Name:	ALKALOID SALTS, SOLID, N.O.S.
14.3	Class(es):	6.1
	Classification code:	T2
	Hazard label(s):	6.1
14.4	Packing group:	III
14.5	Environmental hazards:	No
14.6	Special precautions for user:	
	Hazard identification number (Kemler No.):	60
	tunnel restriction code:	E
		(Passage forbidden through tunnels of category E.)

Sea transport (IMDG)

14.1	UN-No.:	1544
14.2	Proper Shipping Name:	ALKALOIDS SALTS, SOLID, N.O.S.
14.3	Class(es):	6.1
	Classification code:	
	Hazard label(s):	6.1
14.4	Packing group:	III
14.5	Environmental hazards:	No
	MARINE POLLUTANT:	No
14.6	Special precautions for user:	
	Segregation group:	-
	EmS-No.	F-A S-A
14.7	Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	
	not relevant	

Air transport (ICAO-TI / IATA-DGR)

14.1	UN-No.:	1544
14.2	Proper Shipping Name:	ALKALOIDS SALTS, SOLID, N.O.S.
14.3	Class(es):	6.1
	Classification code:	
	Hazard label(s):	6.1
14.4	Packing group:	III
14.5	Special precautions for user:	

SECTION 15: Regulatory information

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

EU legislation

- 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 (Text with EEA relevance)
- Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance)
- Commission Regulation (EU) No 453/2010 of 20 May 2010 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (Text with EEA relevance)
- Commission Regulation (EU) 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

National regulations

no data available

Water hazard class (WGK): slightly hazardous to water (WGK 1)

15.2 Chemical Safety Assessment

not relevant



SECTION 16: Other information

Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists

ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road

AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)

CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures

DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)

Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)

IATA-DGR - International Air Transport Association-Dangerous Goods Regulations

ICAO-TI - International Civil Aviation Organization-Technical Instructions

IMDG - International Maritime Code for Dangerous Goods

LTV - Long Term Value

NIOSH - National Institute for Occupational Safety and Health

OSHA - Occupational Safety & Health Administration

PBT - Persistent, Bioaccumulative and Toxic

RID - Regulation concerning the International Carriage of Dangerous Goods by Rail

STV - Short Term Value

SVHC - Substances of Very High Concern

vPvB - very Persistent, very Bioaccumulative

Additional information

Indication of changes: general update

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.