

Chemical Safety Data Sheet MSDS / SDS

L-Valine, 3-methyl-N-[[1-(4-penten-1-yl)-1H-indazol-3-yl]carbonyl]-, methyl ester

Revision Date:2026-05-31 Revision Number:1

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

Product name : L-Valine, 3-methyl-N-[[1-(4-penten-1-yl)-1H-indazol-3-yl]carbonyl]-, methyl ester
CBnumber : CB88218119
CAS : 2504100-70-1
Synonyms : MDMB-4en-PINACA,Unii-K2dzn2td6

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.
P312 Call a POISON CENTER or doctor/physician if you feel unwell.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.
P330 Rinse mouth.
P501 Dispose of contents/container to.....
P280 Wear protective gloves/protective clothing/eye protection/face protection.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P312 Call a POISON CENTER or doctor/physician if you feel unwell.

P322 Specific measures (see ...on this label).

P363 Wash contaminated clothing before reuse.

P501 Dispose of contents/container to.....

Hazard statements

H302 Harmful if swallowed

H312 Harmful in contact with skin

H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: L-Valine, 3-methyl-N-[[1-(4-penten-1-yl)-1H-indazol-3-yl]carbonyl]-, methyl ester
Synonyms	: MDMB-4en-PINACA, Unii-K2dzn2tdd6
CAS	: 2504100-70-1
MF	: C20H27N3O3
MW	: 357.45

SECTION 4: First aid measures

Description of first aid measures

General information

Immediately remove any clothing soiled by the product.

Remove breathing apparatus only after contaminated clothing have been completely removed.

In case of irregular breathing or respiratory arrest provide artificial respiration.

After inhalation

Supply fresh air or oxygen; call for doctor.

In case of unconsciousness place patient stably in side position for transportation.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

After eye contact

Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing

Do not induce vomiting; immediately call for medical help.

Most important symptoms and effects, both acute and delayed

No further relevant information available.

Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing agents

CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

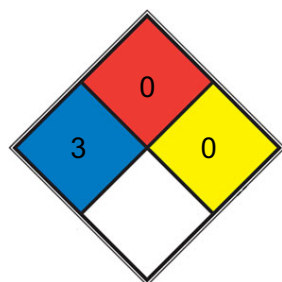
67-56-1 During heating or in case of fire poisonous gases are produced.

Advice for firefighters

Protective equipment

Mouth respiratory protective device.

NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Mount respiratory protective device.

Wear protective equipment. Keep unprotected persons away.

Environmental precautions

Dilute with plenty of water.

Do not allow to enter sewers/ surface or ground water.

Methods and material for containment and cleaning up

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Dispose contaminated material as waste according to section 13.

Ensure adequate ventilation.

Protective Action Criteria for Chemicals

PAC-1

67-56-1 Methanol 530 ppm

PAC-2

67-56-1 Methanol 2,100 ppm

PAC-3

67-56-1 Methanol 7200* ppm

Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

Precautions for safe handling

Ensure good ventilation/exhaustion at the workplace.

Open and handle receptacle with care.

Prevent formation of aerosols.

Information about protection against explosions and fires

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

Keep respiratory protective device available.

Conditions for safe storage, including any incompatibilities

Storage

Store in accordance with information listed on the product insert.

Requirements to be met by storerooms and receptacles

Store in a cool location.

Information about storage in one common storage facility

Not required.

Further information about storage conditions

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

Specific end use(s)

No further relevant information available.

SECTION 8: Exposure controls/personal protection

Control parameters

Components with limit values that require monitoring at the workplace:

67-56-1 Methanol	
PEL	Long-term value: 260 mg/m ³ , 200 ppm
REL	Short-term value: 325 mg/m ³ , 250 ppm
	Long-term value: 260 mg/m ³ , 200 ppm
	Skin
TLV	Short-term value: 250 ppm
	Long-term value: 200 ppm
	Skin; BElc

Ingredients with biological limit values:	
67-56-1 Methanol	
BEI	15 mg/L
	Medium: urine
	Time: end of shift
	Parameter: Methanol (background, nonspecific)

Additional information

The lists that were valid during the creation were used as basis.

Exposure controls

Appropriate engineering controls

No further data; see section 7.

Personal protective equipment

General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Avoid contact with the eyes and skin.

Breathing equipment

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

Protection of hands

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection

Tightly sealed goggles

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State

Liquid

Color

According to product specification

Odor

Alcohol-like

Structural Formula

C₂₀H₂₇N₃O₃

Molecular Weight

357.5 g/mol

Storage Buffer

Odor Threshold

Not determined.

Formulation

A 1 mg/ml solution in methanol

Melting point/Melting range

-98 °C (-144.4 °F)

Boiling point/Boiling range

64.7 °C (148.5 °F)

Flammability

Highly flammable.

Explosion limits

Lower: 5.5 Vol %

Upper: 44 Vol %

Flash point

11 °C (51.8 °F)

Auto igniting

455 °C (851 °F)

Decomposition temperature

Not determined.

pH

Not determined.

Viscosity**Kinematic**

Not determined.

SOLUBILITY

DMF: 12 mg/ml; DMSO: 12 mg/ml; DMSO:PBS (pH 7.2)(1:8): 0.11 mg/ml; Ethanol: 10 mg/ml

Dynamic

Not determined.

Solubility in / Miscibility with

DMF: 12 mg/ml; DMSO: 12 mg/ml; DMSO:PBS (pH 7.2)(1:8): 0.11 mg/ml; Ethanol: 10 mg/ml

Water at 20 °C (68 °F)

1000 g/l

Partition coefficient (n-octanol/water)

Not determined.

Vapor Pressure at 20 °C (68 °F)

128 hPa (96 mm Hg)

Density at 20 °C (68 °F)

0.79 g/cm³ (6.59255 lbs/gal)

Relative Density

1.11±0.1 g/cm³(Predicted)

Vapor Density

Not determined.

Particle characteristics

Not applicable.

Other information

Appearance

Form

Liquid

Important information on protection of health and environment, and on safety.

Ignition temperature

Product is not selfigniting.

Danger of explosion

Product is not explosive. However, formation of explosive air/vapor mixtures are possible.

Organic solvents

99.9 %

VOC content

99.90 % 999.0 g/l / 8.34 lb/gal

Solids content

0.0 %

Change in condition

Evaporation Rate

Not determined.

SECTION 10: Stability and reactivity

Reactivity

No further relevant information available.

Chemical stability

Thermal decomposition / conditions to be avoided

No decomposition if used according to specifications.

Possibility of hazardous reactions

No dangerous reactions known.

Conditions to avoid

No further relevant information available.

Incompatible materials

No further relevant information available.

Hazardous decomposition products

No dangerous decomposition products known.

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD/LC50 values that are relevant for classification:

Substance / Estimate	Route	Endpoint	Value
ATE (Acute Toxicity Estimate)	Oral	LD50	100 mg/kg (rat)
ATE (Acute Toxicity Estimate)	Dermal	LD50	300 mg/kg (rabbit)
ATE (Acute Toxicity Estimate)	Inhalative	LC50/4 h	3.1 mg/l (rat)
67-56-1 Methanol	Oral	LD50	100.1 mg/kg (rat) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Symptoms: Nausea, Vomiting
67-56-1 Methanol	Dermal	LD50	300.1 mg/kg (rabbit) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
67-56-1 Methanol	Inhalative	LC50/4 h	3.1 mg/l (rat) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Symptoms: Irritation symptoms in the respiratory tract.

Primary irritant effect

on the skin

No irritant effect.

on the eye

No irritating effect.

Sensitization

No sensitizing effects known.

Additional toxicological information

The product shows the following dangers according to internally approved calculation methods for preparations

Toxic

Interactive effects

No interactive effects between components are known.

Carcinogenic categories

IARC (International Agency for Research on Cancer)

None of the ingredients is listed.

NTP (National Toxicology Program)

None of the ingredients is listed.

OSHA-Ca (Occupational Safety & Health Administration)

None of the ingredients is listed.

Alternative sources for toxicological information

No non-standard sources for toxicological information where used.

SECTION 12: Ecological information

Toxicity

Aquatic toxicity

No further relevant information available.

Persistence and degradability

No further relevant information available.

Bioaccumulative potential

No further relevant information available.

Mobility in soil

No further relevant information available.

Results of PBT and vPvB assessment

PBT

Not applicable.

vPvB

Not applicable.

PBT:

Not applicable.

vPvB:

Not applicable.

Other adverse effects

Additional ecological information

General notes

Water hazard class 2 (Self-assessment) hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

SECTION 13: Disposal considerations

Waste treatment methods

Recommendation

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

Uncleaned packagings

Recommendation

Disposal must be made according to official regulations.

Recommended cleansing agent

Water, if necessary with cleansing agents.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA UN1230

UN proper shipping name

DOT, IATA Methanol

IMDG METHANOL

Transport hazard class(es)

DOT

Class: 3 Flammable liquids

Label: 3, 6.1

IMDG

Class: 3 Flammable liquids

Label: 3/6.1

IATA

Class: 3 Flammable liquids

Label: 3 (6.1)

Packing group

DOT, IMDG, IATA II

Environmental hazards

Not applicable.

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable.

Transport/Additional information

DOT:

Quantity limitations

On passenger aircraft/rail: 1 L

On cargo aircraft only: 60 L

IMDG:

Limited quantities (LQ)

1L

Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

IATA:

Remarks

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

Special precautions for user

Warning: Flammable liquids

Hazard identification number (Kemler code)

336

EMS Number

F-E, S-D

Stowage Category

B

Stowage Code

SW2 Clear of living quarters.

UN "Model Regulation"

UN 1230 METHANOL, 3 (6.1), II

SECTION 15: Regulatory information

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

No further relevant information available.

Sara

Section 355 (extremely hazardous substances):	None of the ingredients is listed.
Section 313 (Specific toxic chemical listings):	67-56-1 Methanol
TSCA (Toxic Substances Control Act):	67-56-1 Methanol ACTIVE
Hazardous Air Pollutants 67-56-1 Methanol	
Chemicals known to cause cancer:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for females:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for males:	None of the ingredients is listed.
Chemicals known to cause developmental toxicity:	67-56-1 Methanol

Carcinogenic categories

EPA (Environmental Protection Agency):	None of the ingredients is listed.
--	------------------------------------

TLV (Threshold Limit Value)

None of the ingredients is listed.

NIOSH-Ca (National Institute for Occupational Safety and Health)

None of the ingredients is listed.

Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

BEI: Biological Exposure Limit

Flammable liquids 2: Flammable liquids – Category 2

Acute toxicity - oral 3: Acute toxicity – Category 3

Specific target organ toxicity (single exposure) 1: Specific target organ toxicity (single exposure) – Category 1

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.