

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Issue date: 01/26/2021 Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form : Mixture

Product name : Custom Acid Surrogate

AL0-130814 Product code

1.2. Recommended use and restrictions on use

: Certified reference material for laboratory use only Use of the substance/mixture

Phenova

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1.4. Emergency telephone number

Emergency number : ChemTel Assistance (US/Canada) 1-800-255-3924

ChemTel Assistance (International) +1 813-248-0585

SECTION 2: Hazard(s) identification

GHS US classification

Flammable liquids H225 Highly flammable liquid and vapor

Category 2

Acute toxicity (oral) H301 Toxic if swallowed

Category 3

Acute toxicity (dermal) H311 Toxic in contact with skin

Category 3

Skin corrosion/irritation H315 Causes skin irritation Category 2

Serious eye damage/eye H319 Causes serious eye irritation

irritation Category 2

Germ cell mutagenicity Suspected of causing genetic defects H341 Category 2

Specific target organ H370

toxicity (single exposure)

Category 1

Specific target organ H373

toxicity (repeated exposure)

Category 2

Full text of H statements: see section 16

GHS Label elements, including precautionary statements **GHS US labeling**

Hazard pictograms (GHS US)





Causes damage to organs



May cause damage to organs through prolonged or repeated exposure



Signal word (GHS US) : Danger

Hazard statements (GHS US) : H225 - Highly flammable liquid and vapor

H301+H311 - Toxic if swallowed or in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eve irritation

H341 - Suspected of causing genetic defects

H370 - Causes damage to organs

H373 - May cause damage to organs through prolonged or repeated exposure

Precautionary statements (GHS US) : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No

smoking.

P233 - Keep container tightly closed.

P260 - Do not breathe dust/fume/gas/mist/vapors/spray.

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P270 - Do not eat, drink or smoke when using this product.

P280 - Wear protective gloves/protective clothing/eye protection/face protection.

P301+P310 - If swallowed: Immediately call a poison center or doctor.

P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse

skin with water/shower.

P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove

contact lenses, if present and easy to do. Continue rinsing.

P308+P313 - If exposed or concerned: Get medical advice/attention.

P314 - Get medical advice/attention if you feel unwell.

P332+P313 - If skin irritation occurs: Get medical advice/attention. P337+P313 - If eye irritation persists: Get medical advice/attention. P362+P364 - Take off contaminated clothing and wash it before reuse.

P370+P378 - In case of fire: Use media other than water to extinguish.

P403+P235 - Store in a well-ventilated place. Keep cool.

P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

Substances

Not applicable

3.2. Mixtures

Name	Product identifier	Conc.
methanol (Component)	(CAS-No.) 67-56-1	96
2-Chlorophenol-d4 (Component)	(CAS-No.) 93951-73-6	1
Phenol (Component)	(CAS-No.) 13127-88-3	1
2,4,6-tribromophenol (Component)	(CAS-No.) 118-79-6	1

Full text of hazard classes and H-statements : see section 16

SECTION 4: First-aid measures

4.1.	Description	of first aid	measures

First-aid measures general : Never give anything by mouth to an unconscious person. Call a POISON CENTER or

doctor/physician. IF exposed or concerned: Get medical advice/attention.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing.

Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing. First-aid measures after skin contact

Immediately call a poison center or doctor/physician. Wash with plenty of soap and water.

Wash contaminated clothing before reuse.

Remove contact lenses, if present and easy to do. Continue rinsing. Rinse cautiously with First-aid measures after eye contact water for several minutes. Obtain medical attention if pain, blinking or redness persists.

First-aid measures after ingestion Rinse mouth. Do NOT induce vomiting. Obtain emergency medical attention. Immediately call a

poison center or doctor/physician.

(acute and delayed) Most important symptoms and effects

Potential Adverse human health effects and symptoms

: Toxic if swallowed. Toxic in contact with skin.

Symptoms/effects after skin contact Repeated exposure to this material can result in absorption through skin causing significant

health hazard. Toxic in contact with skin.

Symptoms/effects after ingestion Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard

Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

Suitable (and unsuitable) extinguishing media

: Use extinguishing media appropriate for surrounding fire. Suitable extinguishing media

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Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Specific hazards arising from the chemical

Fire hazard : Highly flammable liquid and vapor.

Explosion hazard : May form flammable/explosive vapor-air mixture.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions : Use water spray or fog for cooling exposed containers. Exercise caution when fighting any

chemical fire. Prevent fire-fighting water from entering environment.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Avoid breathing dust/fume/gas/mist/vapors/spray.

Emergency procedures : Ventilate area

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up in absorbent material. Collect spillage.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.

Precautions for safe handling : Wash hands and other exposed areas with mild soap and water before eating, drinking or

smoking and when leaving work. Provide good ventilation in process area to prevent formation

of vapor. No open flames. No smoking. Use only non-sparking tools.

Hygiene measures : Do not eat, drink or smoke when using this product. Gently wash with plenty of soap and water.

Remove/Take off immediately all contaminated clothing. Wash contaminated clothing before

reuse.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Ground/bond

container and receiving equipment.

Storage conditions : Keep in fireproof place. Keep container tightly closed. Keep container tightly closed and in a

well-ventilated place. Keep away from any flames or sparking source.

Incompatible materials : Direct sunlight. Heat sources.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Custom Acid Surrogate		
ACGIH	Local name	Methanol
ACGIH	ACGIH TWA (ppm)	200 ppm
ACGIH	ACGIH STEL (ppm)	250 ppm
ACGIH	Remark (ACGIH)	Headache; eye dam; dizziness; nausea
ACGIH	Regulatory reference	ACGIH 2018
OSHA	OSHA PEL (TWA) (mg/m³)	260 mg/m³
OSHA	OSHA PEL (TWA) (ppm)	200 ppm
OSHA	Regulatory reference (US-OSHA)	OSHA

2-Chlorophenol-d4 (93951-73-6)

Not applicable

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methanol (67-56-1)			
ACGIH	Local name	Methanol	
ACGIH	ACGIH TWA (ppm)	200 ppm (Methanol; USA; Time-weighted average exposure limit 8 h; TLV - Adopted Value)	
ACGIH	ACGIH STEL (ppm)	250 ppm (Methanol; USA; Short time value; TLV - Adopted Value)	
ACGIH	Remark (ACGIH)	Headache; eye dam; dizziness; nausea	
ACGIH	Regulatory reference	ACGIH 2018	
OSHA	OSHA PEL (TWA) (mg/m³)	260 mg/m³	
OSHA	OSHA PEL (TWA) (ppm)	200 ppm	
OSHA	Regulatory reference (US-OSHA)	OSHA	
Phenol (13127-88-3)			
ACGIH	ACGIH TWA (ppm)	5 ppm (Phenol; USA; Time-weighted average exposure limit 8 h; TLV - Adopted Value)	
2,4,6-tribromophenol (118-79-6)			
ACGIH	ACGIH TWA (mg/m³)	3 mg/m³ (Respirable fraction)	

8.2. Appropriate engineering controls

Appropriate engineering controls : Either local exhaust or general room ventilation is usually required.

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Avoid all unnecessary exposure. Gloves. Protective clothing. Protective goggles. Safety glasses.

Hand protection:

Wear chemically resistant protective gloves. Wear suitable gloves resistant to chemical penetration

Eye protection:

Chemical goggles or safety glasses. Safety glasses

Skin and body protection:

Wear chemically protective gloves, lab coat or apron to prevent prolonged or repeated skin contact

Respiratory protection:

Where exposure through inhalation may occur from use, respiratory protection equipment is recommended

Personal protective equipment symbol(s):







Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic	physical and chemical properties	
Physical state	: Liquid	
	: Colorless	
	: characteristic	
Odor threshold	: No data available	
рН	: No data available	
Melting point	: No data available	
Freezing point	: No data available	
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Boiling point : No data available
Flash point : No data available
Relative evaporation rate (butyl acetate=1) : No data available

Flammability (solid, gas) : Highly flammable liquid and vapor.

Vapor pressure : No data available Relative vapor density at 20 °C : No data available Relative density : No data available Solubility : No data available Partition coefficient n-octanol/water (Log Pow) : No data available : No data available Auto-ignition temperature Decomposition temperature : No data available Viscosity, kinematic : No data available : No data available Viscosity, dynamic **Explosion limits** : No data available : No data available Explosive properties : No data available Oxidizing properties

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Highly flammable liquid and vapor. May form flammable/explosive vapor-air mixture.

10.3. Possibility of hazardous reactions

Not established.

10.4. Conditions to avoid

Direct sunlight. Extremely high or low temperatures. Open flame.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

May release flammable gases.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Custom Acid Surrogate			
ATE US (oral)	102.881 mg/kg body weight		
ATE US (dermal)	309.278 mg/kg body weight		
2-Chlorophenol-d4 (93951-73-6)			
LD50 oral rat	670 mg/kg		
ATE US (oral)	670 mg/kg body weight		
methanol (67-56-1)			
LD50 oral rat	> 5000 mg/kg (Rat; BASF test; Literature study; 1187-2769 mg/kg bodyweight; Rat; Weight of evidence)		
LD50 dermal rabbit	15800 mg/kg (Rabbit; Literature study)		
LC50 inhalation rat (mg/l)	85 mg/l/4h (Rat; Literature study)		
LC50 inhalation rat (ppm)	64000 ppm/4h (Rat; Literature study)		
ATE US (oral)	100 mg/kg body weight		
ATE US (dermal)	300 mg/kg body weight		
ATE US (gases)	700 ppmV/4h		
ATE US (vapors)	3 mg/l/4h		

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methanol (67-56-1)			
ATE US (dust, mist)	0.5 mg/l/4h		
Phenol (13127-88-3)			
ATE US (oral)	100 mg/kg body weight		
ATE US (dermal)	300 mg/kg body weight		
ATE US (gases)	700 ppmV/4h		
ATE US (vapors)	3 mg/l/4h		
ATE US (dust, mist)	0.5 mg/l/4h		
2,4,6-tribromophenol (118-79-6)			
LD50 oral rat	2000 mg/kg (Rat, Oral)		
LD50 dermal rabbit	> 8000 mg/kg (Rabbit, Dermal)		
ATE US (oral)	2000 mg/kg body weight		
Skin corrosion/irritation	: Causes skin irritation.		
Serious eye damage/irritation	: Causes serious eye irritation.		
Respiratory or skin sensitization	: Not classified		
Germ cell mutagenicity	: Suspected of causing genetic defects.		
	Based on available data, the classification criteria are not met		
Carcinogenicity	: Not classified		
Phenol (13127-88-3)			
IARC group	3 - Not classifiable		
Reproductive toxicity	: Not classified		
,	Based on available data, the classification criteria are not met		
STOT-single exposure	: Causes damage to organs.		
STOT-repeated exposure	: May cause damage to organs through prolonged or repeated exposure.		
Aspiration hazard	: Not classified		
Potential Adverse human health effects and	: Toxic if swallowed. Toxic in contact with skin.		
symptoms			
Symptoms/effects after skin contact	: Repeated exposure to this material can result in absorption through skin causing significant health hazard. Toxic in contact with skin.		
Symptoms/effects after ingestion	: Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard.		

SECTION 12: Ecological information

12.1. Toxicity

2-Chlorophenol-d4 (93951-73-6)			
LC50 fish 1	6 – 16 mg/l Pimephales promelas (fathead minnow)		
EC50 Daphnia 1	6.3 – 17.9 mg/l Daphnia magna (water flea)		
LC50 fish 2	10.7 – 15.2 mg/l Carassius auratus (goldfish)		
methanol (67-56-1)			
LC50 fish 1	15400 mg/l (LC50; EPA 660/3 - 75/009; 96 h; Lepomis macrochirus; Flow-through system; Fresh water; Experimental value)		
EC50 Daphnia 1	> 10000 mg/l (EC50; DIN 38412-11; 48 h; Daphnia magna; Static system; Fresh water; Experimental value)		
LC50 fish 2	10800 mg/l (LC50; 96 h; Salmo gairdneri)		

12.2. Persistence and degradability

Custom Acid Surrogate	
Persistence and degradability	Not established.
methanol (67-56-1)	
Persistence and degradability	Readily biodegradable in water. Biodegradable in the soil. Highly mobile in soil.

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Custom Acid Surrogate

methanol (67-56-1)

2-Chlorophenol-d4 (93951-73-6)

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methanol (67-56-1)			
Biochemical oxygen demand (BOD)	0.6 – 1.12 g O₂/g substance		
Chemical oxygen demand (COD)	1.42 g O₂/g substance		
ThOD	1.5 g O₂/g substance		
BOD (% of ThOD)	0.8 (Literature study)		
Phenol (13127-88-3)			
Persistence and degradability	Readily biodegradable in water. Biodegradable in the soil. Inhibits biodegradation processes in the soil.		
Biochemical oxygen demand (BOD)	1.68 g O₂/g substance		
Chemical oxygen demand (COD)	2.28 g O₂/g substance		
ThOD	2.38 g O₂/g substance		
BOD (% of ThOD)	0.71		
2,4,6-tribromophenol (118-79-6)			
Persistence and degradability	Biodegradability in soil: no data available. Not readily biodegradable in water.		
2.3. Bioaccumulative potential			
Custom Acid Surrogate			
Bioaccumulative potential	Not established.		
methanol (67-56-1)			
BCF fish 1	< 10 (BCF; 72 h; Leuciscus idus)		
Partition coefficient n-octanol/water (Log Pow)	-0.77 (Experimental value; Other)		
Bioaccumulative potential	Low potential for bioaccumulation (BCF < 500).		
Phenol (13127-88-3)			
BCF fish 1	20 (BCF)		
BCF fish 2	1276 – 1496 (BCF)		
BCF other aquatic organisms 1	277 (BCF)		
BCF other aquatic organisms 2	3.5 – 16 (BCF)		
Partition coefficient n-octanol/water (Log Pow)	1.46 (Experimental value)		
Bioaccumulative potential	Potential for bioaccumulation (500 ≤ BCF ≤ 5000).		
2,4,6-tribromophenol (118-79-6)			
	1.00 (00.17)		
Partition coefficient n-octanol/water (Log Pow)	4.02 (QSAR)		
Partition coefficient n-octanol/water (Log Pow) Bioaccumulative potential	4.02 (QSAR) No bioaccumulation data available.		
` ` ` `			
Bioaccumulative potential 2.4. Mobility in soil			
Bioaccumulative potential			

Phenol (13127-88-3)	
2.4.4.11	
2,4,6-tribromophenol (118-79-6)	

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Other information · Avoid release to the environment

SECTION 13: Disposal considerations

13.1. Disposal methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Additional information : Handle empty containers with care because residual vapors are flammable.

Ecology - waste materials : Avoid release to the environment. Hazardous waste due to toxicity.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN1992 Flammable liquids, toxic, n.o.s. (methanol), 3 (6.1), II

UN-No.(DOT) · UN1992

Proper Shipping Name (DOT) Flammable liquids, toxic, n.o.s.

methanol

Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120

Packing group (DOT) : II - Medium Danger

: 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132 Subsidiary risk (DOT)

Hazard labels (DOT) 3 - Flammable liquid

6.1 - Poison



: 202 DOT Packaging Non Bulk (49 CFR 173.xxx) DOT Packaging Bulk (49 CFR 173.xxx) : 243

DOT Special Provisions (49 CFR 172.102)

: IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized.

T7 - 4 178.274(d)(2) Normal...... 178.275(d)(3)

TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.

TP13 - Self-contained breathing apparatus must be provided when this hazardous material is

transported by sea.

DOT Packaging Exceptions (49 CFR 173.xxx) DOT Quantity Limitations Passenger aircraft/rail : 1 L

(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 60 L

CFR 175.75)

: B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a **DOT Vessel Stowage Location**

passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this

section is exceeded.

DOT Vessel Stowage Other : 40 - Stow "clear of living quarters"

Emergency Response Guide (ERG) Number : 131

Other information : No supplementary information available.

Transportation of Dangerous Goods

Not applicable

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Transport by sea

Transport document description (IMDG) : UN 1992 FLAMMABLE LIQUID, TOXIC, N.O.S. (methanol), 3 (6.1), II

UN-No. (IMDG) : 1992

Proper Shipping Name (IMDG) : FLAMMABLE LIQUID, TOXIC, N.O.S.

Class (IMDG) : 3 - Flammable liquids

Packing group (IMDG) : II - substances presenting medium danger

Subsidiary risks (IMDG) : 6.1 - Toxic substances

Limited quantities (IMDG) : 1 L

Air transport

Transport document description (IATA) : UN 1992 Flammable liquid, toxic, n.o.s. (methanol), 3 (6.1), II

: 6.1 - Toxic substances

UN-No. (IATA) : 1992

Proper Shipping Name (IATA) : Flammable liquid, toxic, n.o.s.

Class (IATA) : 3 - Flammable Liquids

Packing group (IATA) : II - Medium Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

Subsidiary hazards (IATA)

2-Chlorophenol-d4 (93951-73-6)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

methanol (67-56-1)

Listed on the United States TSCA (Toxic Substances Control Act) inventory Subject to reporting requirements of United States SARA Section 313

Listed on EPA Hazardous Air Pollutant (HAPS)

CERCLA RQ 5000 lb

Phenol (13127-88-3)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

2,4,6-tribromophenol (118-79-6)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

EPA TSCA Regulatory Flag

T - T - indicates a substance that is the subject of a final TSCA section 4 test rule.

15.2. International regulations

CANADA

2-Chlorophenol-d4 (93951-73-6)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

methanol (67-56-1)

Listed on the Canadian DSL (Domestic Substances List)

Phenol (13127-88-3)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

2,4,6-tribromophenol (118-79-6)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

methanol (67-56-1)

Listed on EPA Hazardous Air Pollutant (HAPS)

15.3. US State regulations

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methanol (67-56-1)					
U.S California - Proposition 65 - Carcinogens List	U.S California - Proposition 65 - Developmental Toxicity	U.S California - Proposition 65 - Reproductive Toxicity - Female	U.S California - Proposition 65 - Reproductive Toxicity - Male	No significant risk level (NSRL)	Maximum allowable dose level (MADL)
No	Yes	No	No		47000 μg/day (inhalation); 23,000 μg/day (oral)

SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE

COUNCIL of 16 December 2008 on classification, labeling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending

Regulation (EC) No 1907/2006.

Other information : None.

Full text of H-phrases:

H225	Highly flammable liquid and vapor
H301	Toxic if swallowed
H311	Toxic in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H341	Suspected of causing genetic defects
H370	Causes damage to organs
H373	May cause damage to organs through prolonged or repeated exposure

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