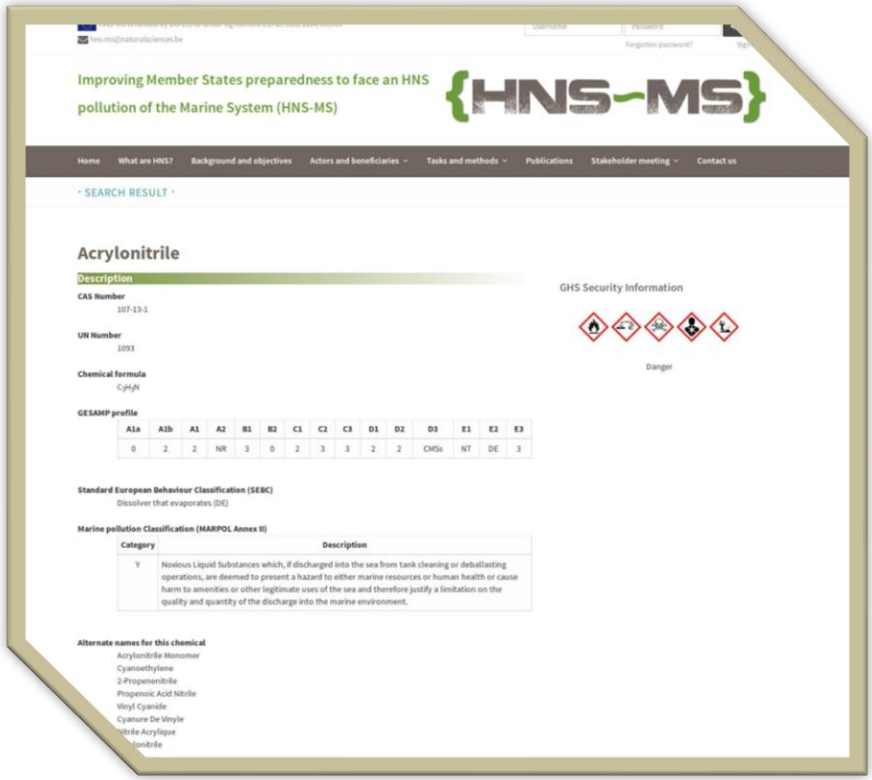
A freely accessible HNS data base



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ARMINES

ALYOTECH

federal public service
HEALTH, FOOD CHAIN SAFETY AND ENVIRONMENT

The HNS data base in a nutshell

- 120 HNS,
  described by 90+ data covering 6 main themes:
  1. Names and regulation
  2. Physical and chemical properties
  3. Behaviour
  4. Ecotoxicity
  5. GESAMP profiles
  6. Hazards

- Searchable through the HNS-MS public website and the HNS-MS private web-application

- Remotely searchable with the public rest API

Data collation

literature review

Lab experiments

Data warehouse

“HNS data base”

Data dissemination

Public website

Private application

Public API

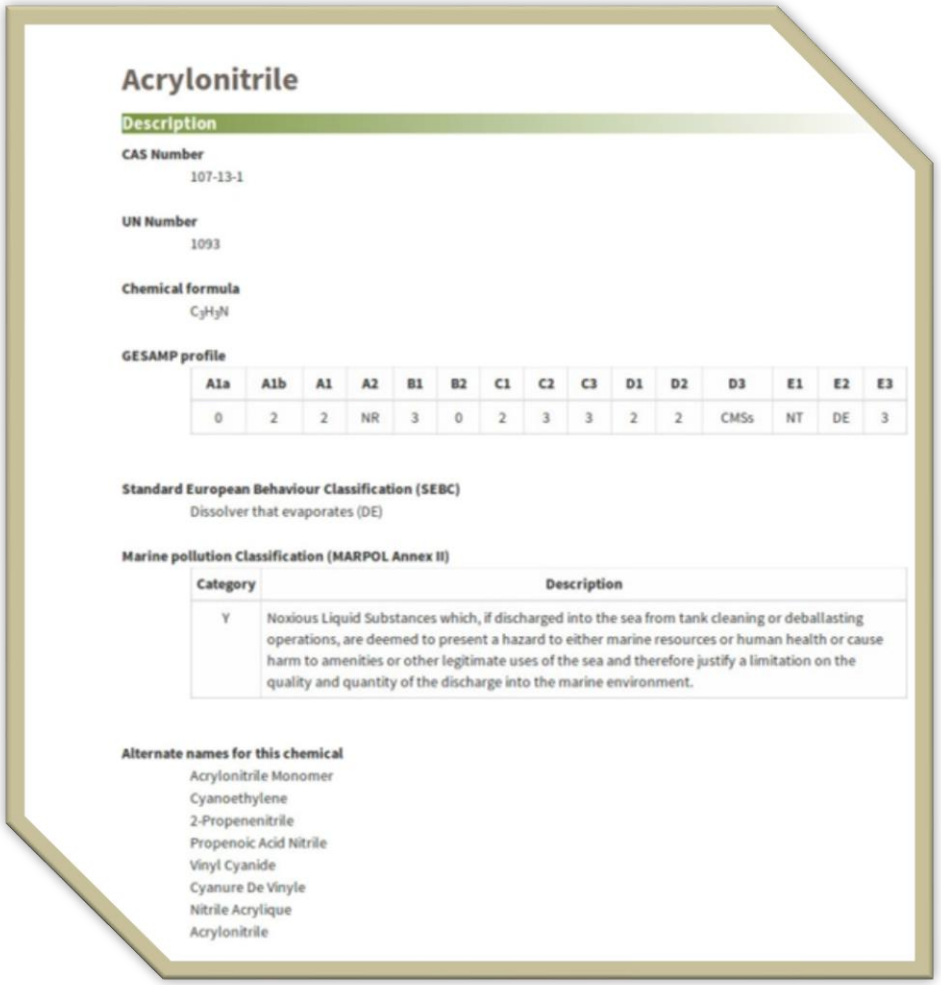
Co-funded by the European Commis

120 HNS

1,2,3-Trichlorobenzene (molten)	Calcium nitrate solutions (50% or less)	Formic acid	Nonylphenol poly (4+)ethoxylate
1,2,4-Trimethylbenzene	Carbon disulphide	Hexamethylenediamine	Octane
1,2-Dichloropropane	Chloroacetic acid	Hexamethylenetetramine solutions	Palm oil
1,2-Propylene glycol	Chloroform	Hydrochloric acid	Pentane
1,3-Cyclopentadiene dimer (molten)	Cyclohexane	Hydrogen peroxide	Phenol
1,5,9-cyclododecatriene	Cyclohexanone	Isobutyl alcohol	Phosphoric acid
1-Butanol	Decene	Isopropylbenzene	Polymethylene polyphenyl isocyanate
1-Hexene	Di(2-ethylhexyl)phthalate	Lauric acid	Potassium hydroxide
2,2,4-Trimethyl-1,3-Pentanediol-1-Isobutyrate	Diethylene glycol	Maleic anhydride	Propionic acid
2-Butoxyethanol	Diisononyl phthalate	Marine Diesel Oil	Propylbenzene
2-Ethylhexanoic acid	Dimethylamine solution	Methacrylic acid	Propylene glycol methyl ether
2-Ethylhexyl acrylate	Dimethylformamide	Methanol	Propylene glycol methyl ether acetate
2-Propanol	Diphenylmethane diisocyanate	Methyl acrylate	Propylene oxide
Acetic acid	Dodecene (all isomers)	Methyl ethyl ketone	Sodium hydroxide
Acetic anhydride	Dodecyl alcohol	Methyl isobutyl ketone	Styrene
Acetone	Dodecylbenzene	Methyl methacrylate	Sulfuric acid
Acetone cyanohydrin	Epichlorohydrin	Methyl tert-butyl ether	Sulphur (commercially formed, solid)
Acrylic acid	Ethanol	Methylene chloride	Sulphur (molten)
Acrylonitrile	Ethanolamine	Naphtha (petroleum), hydrodesulfurized heavy	Tall Oil
Adiponitrile	Ethyl acetate	Naphthalene	Tallow
Ammonia anhydrous	Ethyl acrylate	Naphtalene crude molten	tert-Amyl methyl ether
Ammonium hydroxide	Ethyl tert-butyl ether	n-Butyl acetate	tert-Butyl alcohol
Ammonium nitrate solution (93% or less)	Ethylbenzene	n-Butyl acrylate	Tetrachloroethylene
Aniline	Ethylene Dichloride	n-Heptane	Tetrahydrofuran
Benzene	Ethylene glycol	n-Hexane	Toluene
Benzene, C10-C13 Alkyl derivs	Ethylene glycol methyl butyl ether	Nitric acid	Toluene diisocyanate
Benzyl chloride	Ethylene glycol monomethyl ether	Nitrobenzene	Trichloroethylene
Bis(2-ethylhexyl) adipate	Ethylenediamine	n-Nonylphenol (mixed isomers)	Urea
Butylene glycol	Fatty Acid Methyl Esters	Nonene	Vinyl acetate
Calcium lignosulphonate solutions	Formaldehyde solutions (45% or less)	Nonyl alcohol (all isomers)	Vinyl ethyl ether
			Xylene (mixed isomers)

Names and regulation

- English name and synonyms
- CAS number
- UN number
- MARPOL annex 2



Acrylonitrile

Description

CAS Number
107-13-1

UN Number
1093

Chemical formula
C_3H_3N

GESAMP profile

A1a	A1b	A1	A2	B1	B2	C1	C2	C3	D1	D2	D3	E1	E2	E3
0	2	2	NR	3	0	2	3	3	2	2	CMSs	NT	DE	3

Standard European Behaviour Classification (SEBC)
Dissolver that evaporates (DE)

Marine pollution Classification (MARPOL Annex II)

Category	Description
Y	Noxious Liquid Substances which, if discharged into the sea from tank cleaning or deballasting operations, are deemed to present a hazard to either marine resources or human health or cause harm to amenities or other legitimate uses of the sea and therefore justify a limitation on the quality and quantity of the discharge into the marine environment.

Alternate names for this chemical
Acrylonitrile Monomer
Cyanoethylene
2-Propenenitrile
Propenoic Acid Nitrile
Vinyl Cyanide
Cyanure De Vinyle
Nitrile Acrylique
Acrylonitrile

Co-funded by the European Commission, DG-ECHO

Physico-Chemical properties

Physico-chemical properties

- Molecular formula
- Molar mass,
- Physical state,
- Melting and boiling point
- Density
- Surface and interfacial tension
- Viscosity
- Solubility in fresh water and seawater
- Vapour pressure
- Vapour density
- Henry's constant
- Enthalpy of vaporization

Combustion parameters

- Flash point
- Lower and upper explosive limits
- Radiative fraction
- Enthalpy of combustion
- Combustion efficiency

Physico-chemical properties	
Chemical formula	C_3H_3N
Molar mass	53.06 g/mol
State at 25 °C and 1 atm	Liquid
Melting point	-83 °C
Boiling point	77.4 °C
Density	0.81
Surface tension at 20 °C	27.22 mN/m
Surface tension at 25 °C	26.63 mN/m
Kinematic viscosity at 20 °C	0.43 cSt
Kinematic viscosity at 25 °C	0.42 cSt
Solubility in fresh water at 20 °C	79000 mg/l
Vapor pressure at 20 °C	11500 Pa
Vapor pressure at 25 °C	14470 Pa
Vapour density	1.9
Flash point (Pensky-Martens closed cup)	-1 °C
Lower Explosive Limit (LEL)	3 %
Upper Explosive Limit (UEL)	17 %
Enthalpy of vaporization at normal boiling temperature	616000 J/Kg
Enthalpy of combustion	31900000 J/Kg
Combustion efficiency	0.98
Mass flow rate of the combustion surface	0.05 $Kg/(m^2 \cdot s)$
Radiative fraction	0.26
Henry's constant	8.7 $mol/(m^3 \cdot Pa)$

Behaviour

- SEBC
- Log K_{ow}
- Log K_{oc}
- Hydrolyse
- Photolyse
- Biodegradation in estuary
- Biodegradation in marine environment
- BioConcentration factor

Behaviour

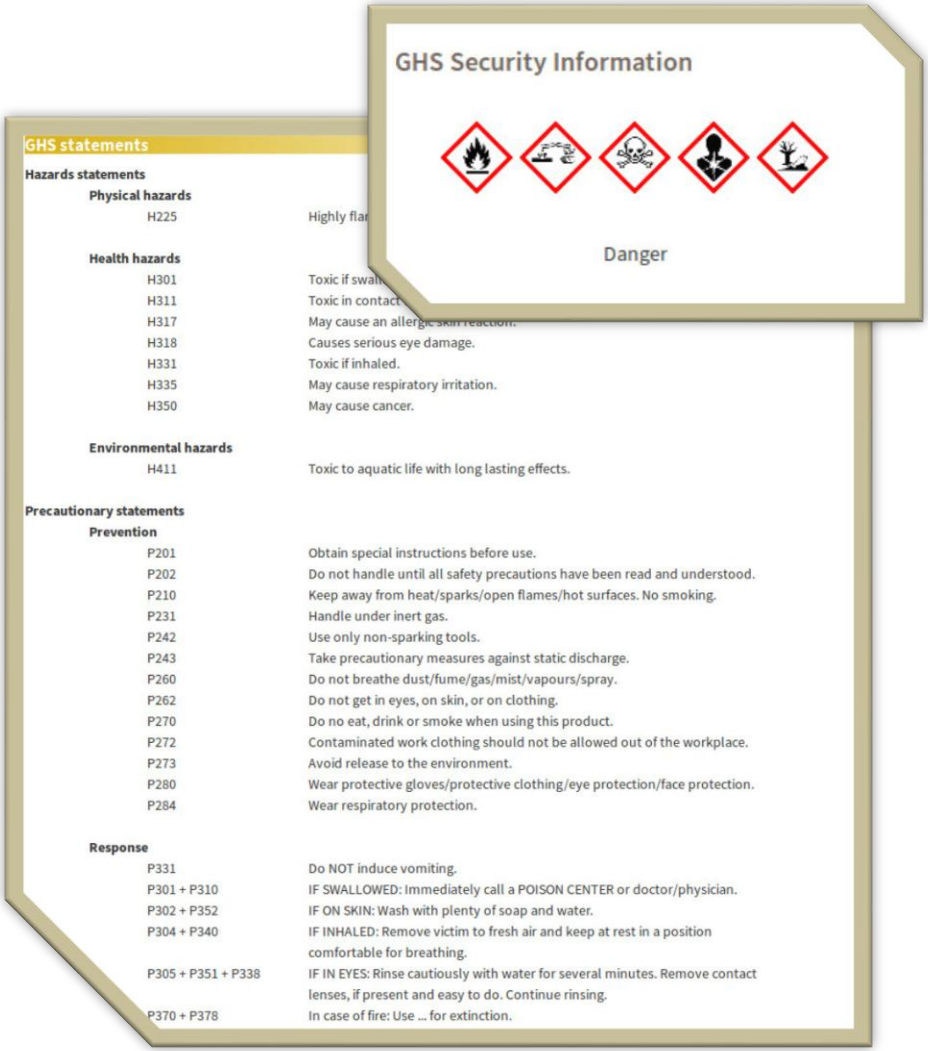
Log Kow	-0.92
Log Koc	-0.07
Hydrolysis (Half-life)	Not hydrolysable
Aqueous photolysis (Half-life)	Not photolysable
Biodegradation in estuary environment (Half-life)	0 day
Biodegradation in marine environment (Half-life)	0 day
Standard European Behaviour Classification (SEBC)	Dissolver that evaporates (DE)
Bioconcentration factor (BCF)	1

GHS / CLP profile

UN Globally Harmonized System for Classification, Labelling and Packaging of Chemicals

- **Hazards statements**
  - Physical hazards (H2xx)
  - Health hazards (H3xx)
  - Environmental hazards (H4xx)

- **Precautionary statements**
  - Prevention (P2xx)
  - Response (P3xx)
  - Storage (P4xx)
  - Disposal (P5xx)



GHS Security Information

Danger

GHS statements

Hazards statements	
Physical hazards	
H225	Highly fla
Health hazards	
H301	Toxic if swal
H311	Toxic in contact
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.
Environmental hazards	
H411	Toxic to aquatic life with long lasting effects.
Precautionary statements	
Prevention	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P231	Handle under inert gas.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P262	Do not get in eyes, on skin, or on clothing.
P270	Do no eat, drink or smoke when using this product.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P284	Wear respiratory protection.
Response	
P331	Do NOT induce vomiting.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P370 + P378	In case of fire: Use ... for extinction.

GHS / CLP profile

UN Globally Harmonized System for Classification, Labelling and Packaging of Chemicals

Health Hazard

- Carcinogen
- Mutagenicity
- Reproductive Toxicity
- Respiratory Sensitizer
- Target Organ Toxicity
- Aspiration Toxicity

Flame

- Flammables
- Pyrophorics
- Self-Heating
- Emits Flammable Gas
- Self-Reactives
- Organic Peroxides

Exclamation Mark

- Irritant (skin and eye)
- Skin Sensitizer
- Acute Toxicity (harmful)
- Narcotic Effects
- Respiratory Tract Irritant
- Hazardous to Ozone Layer (Non Mandatory)

Gas Cylinder

- Gases under Pressure

Corrosion

- Skin Corrosion/ burns
- Eye Damage
- Corrosive to Metals

Exploding Bomb

- Explosives
- Self-Reactives
- Organic Peroxides

Flame over Circle

- Oxidizers

Environment (Non Mandatory)

- Aquatic Toxicity

Skull and Crossbones

- Acute Toxicity (fatal or toxic)

GESAMP hazard profile

GESAMP
Group of Experts on the Scientific Aspects of Marine Environmental Protection

A. Bioaccumulation and biodegradation

B. Aquatic toxicity

C. Acute mammalian toxicity

D. Irritation, corrosion and long-term health effects

E. Inference with other use of the sea

GESAMP

GESAMP hazard profile

A1a	A1b	A1	A2	B1	B2	C1	C2	C3	D1	D2	D3	E1	E2	E
0	2	2	NR	3	0	2	3	3	2	2	CMSs	NT	DE	3

A1: Bioaccumulation

Rating	Description
2	Low potential to bioaccumulate

A1a

Rating	Description	Criteria for log Pow
0	No potential to bioaccumulate	log P <1

A1b

Rating	Description	Criteria for bioconcentration factor
2	Low potential to bioaccumulate	10≤ BCF <100

A2 : Biodegradation

Rating	Description
NR	Not readily biodegradable

B1 : Acute aquatic toxicity

Rating	Description	LC/LL_{50} , EC/EL_{50} , IC/IL_{50} [mg/l]
3	Moderately toxic	1< LC/EC/IC50 ≤10

B2 : Chronic aquatic toxicity

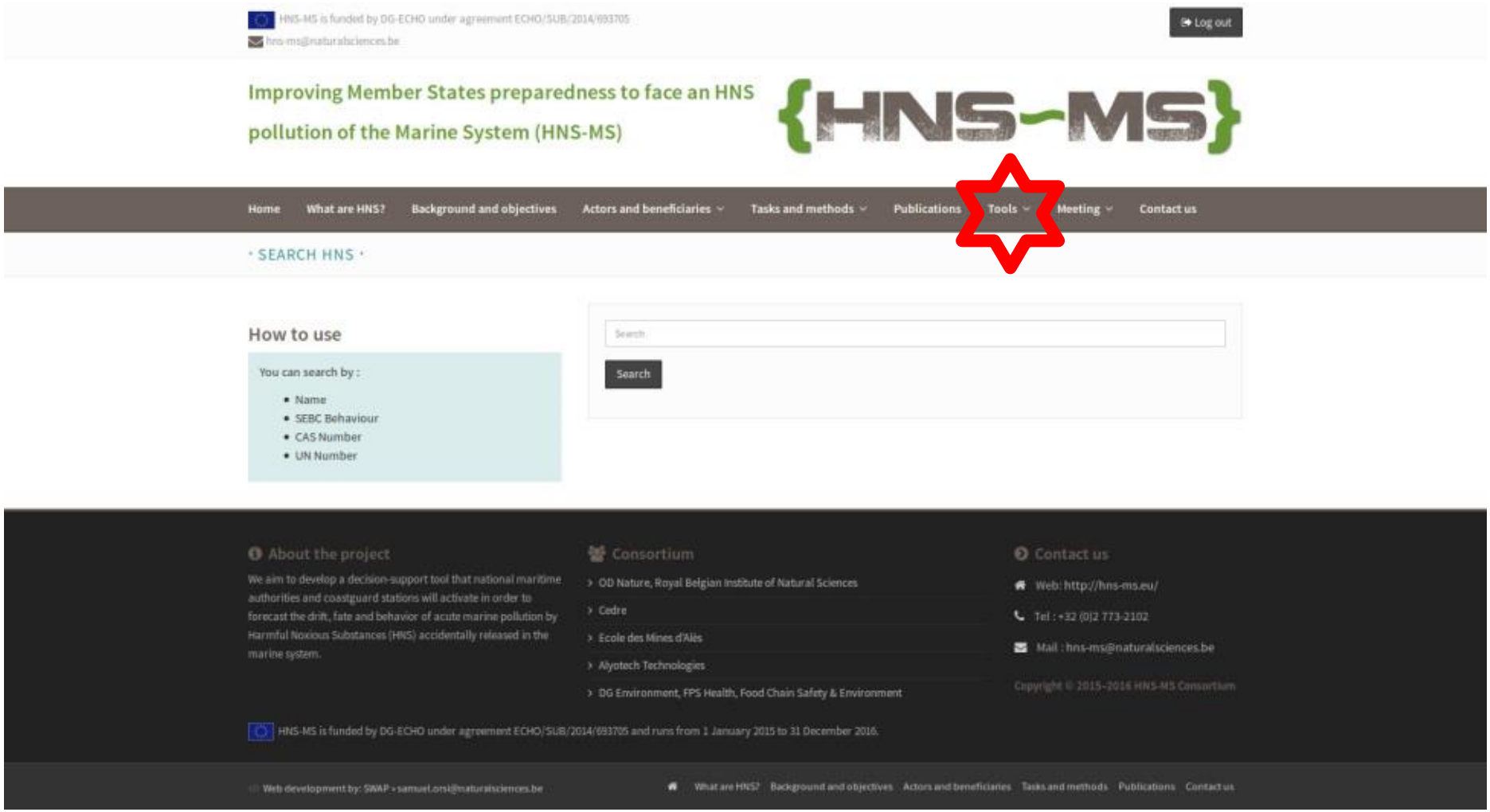
Rating	Description	No observed effect concentration [mg/l]
0	Negligible	1< NOEC

: Acute oral toxicity

ting	Relative Hazard	Acute oral toxicity estimate [mg/kg]

Searchable via HNS-MS public website

http://www.hns-ms.eu/hnsdb/



HNS-MS is funded by DG-ECHO under agreement ECHO/SUB/2014/693705
hns-ms@naturalsciences.be

Log out

Improving Member States preparedness to face an HNS pollution of the Marine System (HNS-MS)

{HNS-MS}

Home | What are HNS? | Background and objectives | Actors and beneficiaries | Tasks and methods | Publications | Tools | Meeting | Contact us

· SEARCH HNS ·

How to use

You can search by :

- Name
- SEBC Behaviour
- CAS Number
- UN Number

107-13

Search

Name	SEBC	CAS Number	UN Number	Details
Acrylonitrile Monomer	DE	107-13-1	1093	Details
Cyanoethylene	DE	107-13-1	1093	Details
2-Propenenitrile	DE	107-13-1	1093	Details
Propenoic Acid Nitrile	DE	107-13-1	1093	Details
Vinyl Cyanide	DE	107-13-1	1093	Details
Cyanure De Vinyle	DE	107-13-1	1093	Details
Nitrile Acrylique	DE	107-13-1	1093	Details
Acrylonitrile	DE	107-13-1	1093	Details

Remotely searchable via a public rest API

- url : https://hns-ms.eu/hnsdb/api/FIELD_TYPE
  - FIELD = search string
  - TYPE = "Name", SEBC, CAS, UN

It returns a json object with all the fields of the HNS that match the search string


```
[{"Name_EN":"Acetic Acid","Name_FR":"Acide
Acetique","CAS_Number":"64-19-7","UN_Number":"2789","Mixed":"0","Formula":"C2H4O2","Molar_Mass":"60.05","Crit_Molar_Volume":null,"State_25_P0":"Liquid","Abilities":null,"Fusion_T":"16
.7","Boiling_T":"117.9","Critical_T":null,"Dens_Liq_20":"1.05","Superficial_Tens_20":null,"Superficial_Tens_25":"27.1","Interfacial_Tens_20":null,"Interfacial_Tens_25":null,"Visco_20"
:"1.16","Visco_25":"1","Hydrosol_FW_20":"1050000","Hydrosol_FW_25":"1050000","Hydrosol_SW_20":null,"Vapor_Pres_20":null,"Vapor_Pres_25":"2093","Critical_Pres":null,"Vapor_Pres_07TCrit
":null,"Vapor_Dens":"1.9","Flash_Point_PMCC":"39.4","Flash_Point_COC":"44.4","Hi_Explos_Limit":"19.9","Lo_Explos_Limit":"4","Vap_Enthalpy_BT":"394670","Vap_Enthalpy_25":"389010","Spec
ific_Heat_25":"2053","Combus_Enthalpy":"13100000","Rad_Fraction":"0.23","Massic_Deb_CS":"0.03","Comb_Efficiency":"0.98","IDLH":"50","Henry_Const":"0.01","Log_Koc":"1.02","Hydrolysis_H
alfLife":"0","Water_Photolysis_HalfLife":"0","Estuary_Biodeg_HalfLife":"10","Marine_Biodeg_HalfLife":"10","Log_Kow":"0.17","Bioconcent_Factor":"1","LC50_Algae_Test_Max":"0","LC50_Alga
e":"20","LC50_Crust_Test_Max":"0","LC50_Crust":"18.9","LC50_Fish_Test_Max":"0","LC50_Fish":"43.8","NOEC_Algae_Test_Max":"0","NOEC_Algae":"10.6","NOEC_Crust_Test_Max":"0","NOEC_Crust":
"22.7","NOEC_Fish_Test_Max":"0","NOEC_Fish":"34.3","Assessement_Factor_ST":"100","PNEC_ST":"189","Assessement_Factor_LT":"100","PNEC_LT":"106","Notable_Risks":"R\u00e9agit avec les
oxydants et les bases fortes","Label_Warning":"Danger","Accident":"0","MarpolCat":"Z","MarpolDes":"Noxious Liquid Substances which, if discharged into the sea from tank cleaning or
deballasting operations, are deemed to present a minor hazard to either marine resources or human health and therefore justify less stringent restrictions on the quality and quantity
of the discharge into the marine environment.","A1ARat":"0","A1ADes":"No potential to bioaccumulate","A1ACri":"log P <1","A1Rat":"0","A1Des":"No potential to
bioaccumulate","A1BRat":"0","A1BDes":"No potential to bioaccumulate","A1BCri":"No measurable bioconcentration factor (BCF)","A2Rat":"R","A2Des":"Readily
biodegradable","B1Rat":"1","B1Des":"Practically non-toxic","B1Cri":"100< LC\/EC\/IC50 \u22641000","B2Rat":"NI","B2Des":"No
Information","B2Cri":null,"C1Rat":"1","C1Des":"Slight","C1Cri":"300< Oral ATE \u22642000","C2Rat":"1","C2Des":"Slight","C2Cri":"1000< Dermal ATE
\u22642000","C3Rat":"1","C3Des":"Slight","C3Cri":"10< Inhalation ATE \u226420","D1Rat":"3C","D1Des":"Corrosive","D1Sign":"Full-thickness skin necrosis following exposure up to 3
min","D1GHS":"Corrosive Category 1A","D2Rat":"3","D2Des":"Severely irritating or corrosive","D2Sign":"Severe conjunctoblepharitis, chemosis, corneal injury or similar effects not
fully reversible within 21 days","D2GHS":"Irritant Category 1","D3":[[null,null,"No Information",null]],"E1Rat":"NI","E1Des":"No
Information","E2Rat":"D","E2Des":"Dissolves","E3Rat":"3","E3Inf":"Highly objectionable","E3Des":"1  is highly acutely toxic; and\/or 2  is severely irritant or corrosive to skin or
eyes; and\/or 3  is carcinogenic, mutagenic or reprotoxic; and\/or 4  is a floater or persistent floater with associated health effects","E3Inp":"1  C1 and\/or C2 and\/or C3 = 4;
and\/or 2  D1 or D2 = 3, 3A, 3B, or 3C; and\/or 3  D3 contains C, M or R; and\/or 4  E2 = F or Fp and D3 contains Ss, Sr, T, A, N, or I","E3War":"Warning issued leading to the
closure of amenities","SEBC":"Dissolves (D)","Syns":["Ethanoic Acid","Ethylic Acid","Methanecarboxylic Acid","Vinegar","Vinegar Acid","Acetic Acid","Acide Acetique","Acetic
Acid","Acide Acetique"],"MDP":[["Physical hazards","H226","Flammable liquid and vapour."]],"MDS":[["Health hazards","H314","Causes severe skin burns and eye damage."]],"CPP":
[["Prevention precautionary statements","P210","Keep away from heat\/sparks\/open flames\/hot surfaces. No smoking."],["Prevention precautionary statements","P241","Use
explosion-proof electrical\/ventilating\/lighting\/...\/equipment."],["Prevention precautionary statements","P260","Do not breathe dust\/fume\/gas\/mist\/vapours\/spray."],
["Prevention precautionary statements","P280","Wear protective gloves\/protective clothing\/eye protection\/face protection."]],"CPI":[["Response precautionary statements","P303 +
P361 + P353","IF ON SKIN (or hair): Remove\/Take off immediately all contaminated clothing. Rinse skin with water\/shower."],["Response precautionary statements","P305 + P351 +
P338","IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing."]],"CPE":[["Disposal precautionary
statements","P501","Dispose of contents\/container to ..."]],"Labeling":[["GHS-SGH02.png","Flammable"],["GHS-SGH05.png","Corrosive"]]},{"Name_EN":"Acetic
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Acetique","CAS_Number":"108-24-7","UN_Number":"1715","Mixed":"0","Formula":"C4H6O3","Molar_Mass":"102.09","Crit_Molar_Volume":null,"State_25_P0":"Liquid","Abilities":null,"Fusion_T":"
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Conclusion

- The HNS data base is the very first **freely accessible** db with 120 HNS,
  - Freely accessible and searchable
  - Specific for marine environment hazard
  - Primary goal: physico-chemical properties to support modelling
  - Contains validated data in not standard T and S conditions, closer to the real field conditions
  - In line with the EU regulation

Interest for MARPOCS MARINER

Perspectives

- Is there missing information that decision makers and/or responders should access?

- How to maintain the database on the long-term?
  - Need for a specific governance?
  - How to add new entries?
  - How to review old ones?
  - How to pay for these service?