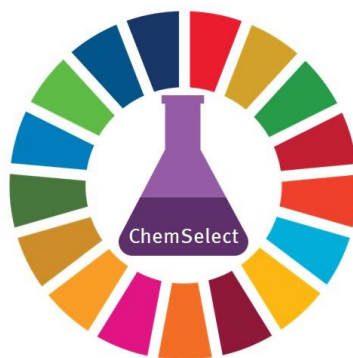


ChemSelect: Example Coolants



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1 Introduction

ChemSelect is an online application that enables formulators and end users of chemicals to assess the sustainability of substances and mixtures. During its development, ChemSelect was tested by various people on many substances and mixtures. This also included comparisons between two products or more that are intended for the same use and differ in their composition. Some of these couples have been selected as examples. They are used in information materials about ChemSelect and also as training material. We use these reports to describe the examples. In these examples, the experiences gained during evaluating the example chemicals are also documented.

To understand the colour scheme: For each criterion, a colour and a number are assigned that indicate the degree of sustainability: **Red**/5 not sustainable; **Green**/1 = sustainable and **yellow**/3 = “in the middle”. If information is missing, the rating is **pink**/4. If no entry has been made for a criterion, it is **grey**/-1. If a criterion is not relevant for a substance or use (e.g. persistent for inorganic substances), a **light blue**/-2 is assigned. Details on the sustainability indicators and the methodology for aggregating the sub-criteria into the main criteria can be found in the evaluation concept.

2 Background information about the products

2.1 Application area and functionality

The evaluated products are gases that are used as coolants, for example in air conditioning systems. Coolants are only handled by professional users; the air conditioning systems can be used commercially or privately. In this example it is assumed that the air conditioning systems containing the coolants are disposed of in Europe and that controlled removal of the coolants is therefore ensured. The evaluation was carried out by the user of the coolant.



2.2 Details about the products

Propane	
Description of the substance	
Name of the substance	Propane
CAS number	74-98-6
EC number	200-827-9
Supplier of the substance	Supplier of gases
<input type="checkbox"/> The substance is a solid at room temperature	
<input checked="" type="checkbox"/> The substance is a gas at room temperature (or boiling point less than 50° C)	
<input type="checkbox"/> The substance is an inorganic substance	

R1234yf (2,3,3,3Tetrafluorpropen)	
Description of the substance	
Name of the substance	R1234yf (2,3,3,3Tetrafluorpropen)
CAS number	754-12-1
EC number	468-710-7
Supplier of the substance	
<input type="checkbox"/> The substance is a solid at room temperature	
<input checked="" type="checkbox"/> The substance is a gas at room temperature (or boiling point less than 50° C)	
<input type="checkbox"/> The substance is an inorganic substance	

The two coolants are supplied by the same supplier. They are both gaseous, so the “slider” at the button is set to blue.

3 Assessment

3.1 Lists of problematic substances

Propane	
Mentioned on problem substance lists	
If marked, the substance was found on a list. The comparison was made automatically using the CAS number.	
✓ Not found on any list by automatic comparison.	
✓ REACH - Candidate List	✓ Stockholm Convention, Persistent Organic Pollutants (POPs)
✓ Substances with high global warming potential	✓ Montreal Protocol, Ozone-depleting substances (ODPs)
✓ List of carcinogens, mutagens and reproductive toxicants (CMR list)	✓ Lists: Substances that can damage the hormone system
Non-regulatory lists	
✓ SIN list	✓ Groups of structurally related substances
<input type="checkbox"/> The substance belongs to a group of chemicals on the candidate list. Please check whether the substance belongs to a group of chemicals listed on the Candidate List without a CAS number.	

R1234yf (2,3,3,3Tetrafluorpropen)	
Mentioned on problem substance lists	
If marked, the substance was found on a list. The comparison was made automatically using the CAS number.	
✓ Not found on any list by automatic comparison.	
✓ REACH - Candidate List	✓ Stockholm Convention, Persistent Organic Pollutants (POPs)
✓ Substances with high global warming potential	✓ Montreal Protocol, Ozone-depleting substances (ODPs)
✓ List of carcinogens, mutagens and reproductive toxicants (CMR list)	✓ Lists: Substances that can damage the hormone system
Non-regulatory lists	
✓ SIN list	✓ Groups of structurally related substances

None of the two substances is included in a list of problematic substances



3.2 Physical-chemical properties

Propane

5 Physico-chemical properties

- 5** H220 - Extremely flammable gas.
- 3** H280 - Contains gas under pressure; may explode if heated.

R1234yf (2,3,3,3Tetrafluorpropen)

3 Physico-chemical properties

- 3** H280 - Contains gas under pressure; may explode if heated.

Both substances can explode when heated. Propane is also flammable. The evaluation is based on the H statements entered.

3.3 Human toxicity

Propane

1 Human toxicity

- 1** Carcinogenic, mutagenic and reproductive toxic effects
- 1** Disruption of the hormonal system in humans
- 1** Damage if in contact with skin and eyes
- 1** Further damage to human health

i Eine gute Quelle zu Eigenschaften von Stoffen ist die Dissimination-Datenbank der ECHA
<https://echa.europa.eu/de/information-on-chemicals>

i The assessment of the human toxicity is based on the hazard statements entered

Disruption of the hormonal system in humans

Disruption of the hormonal system

i The substance's CAS number was compared to several lists (Sin list, TEDX-Colburn EUH381) were checked. You can enter your assessment here with (further) evidence
<https://echa.europa.eu/de/ed-assessment>

R1234yf (2,3,3,3Tetrafluorpropen)

1 Human toxicity

- 1** Carcinogenic, mutagenic and reproductive toxic effects
- 1** Disruption of the hormonal system in humans
- 1** Damage if in contact with skin and eyes
- 1** Further damage to human health

i Eine gute Quelle zu Eigenschaften von Stoffen ist die Dissimination-Datenbank der ECHA
<https://echa.europa.eu/de/information-on-chemicals>

i The assessment of the human toxicity is based on the hazard statements entered

Disruption of the hormonal system in humans

Disruption of the hormonal system

i The substance's CAS number was compared to several lists (Sin list, TEDX-Colburn EUH381) were checked. You can enter your assessment here with (further) evidence
<https://echa.europa.eu/de/ed-assessment>



Both gases are not harmful to humans. Respiratory problems are known for propane at very high inhaled concentrations; however, this does not lead to a classification. Therefore the results for both gases are identical.

R1234yf is broken down in the atmosphere into, among other things, trifluoroacetic acid (TFA) and is washed out of the air with rain. TFA is persistent and very mobile and reaches aquifers, some of which are used as a source of drinking water. The German authorities have submitted an application for a harmonized classification as toxic to reproduction. There is no option to enter information about classification proposals for carcinogenicity, mutagenicity and reprotoxic effects (CMR), but this information should be kept in mind and respective processes be watched.

If the breakdown product of R1234yf will be classified as reprotoxic, the assessment will result in a red mark for the CMR sub-criterion.

3.4 Environmental toxicity

In the evaluation of the environmental toxicity of R1234yf, its degradation to TFA can be taken into account as a category “suspected” or “indications in literature” exist. Although not yet manifesting in a harmonised classification, there are very strong indications of TFA being a PMT or vPvM. Therefore, the option that the literature (already) refers to TFA as a PMT is selected. Trifluoro acetic acid is also classified as H412. This H statement has been inserted for the substance R1234yf as the precursor of TFA.

The “Long-distance transport” parameter is set to “not relevant” as the default, since gases are and remain in the air. Their transport distance primarily depends on their persistence in air, which is considered already in the PBT/vPvB or PMT/vPvM criterion. Long-distance transport is therefore not included in the rating at all.



ChemSelect: Assessment of coolants (gases)

Propane

1

Environmental toxicity

1

 Aquatic toxicity

1

 PBT/vPvB substances and long-distance transport

1

 PMT/vPvM substances

1

 Disruptions of the hormone system in the environment

i The assessment of the environmental toxicity is based on the hazard statements entered at the beginning. In addition, additional sources can be taken into account for various aspects.

☐ This is an inorganic substance

1

Aquatic toxicity

i This criterion is used to assess the acute and chronic toxicity to aquatic organisms.

Relevant H statements No

A There is no classification for aquatic toxicity. Enter data from studies to assess the criterion.

Acute aquatic toxicity (LC50) [mg/l]

Chronic aquatic toxicity (NOEC or EC10) [mg/l]

1

PBT/vPvB substances and long-distance transport

1

PBT/vPvB

Information on PBT properties

No indication of PBT/ vPvB properties

PERSISTENCE

Simulation study: (not recorded) -- Days

Degradability: Not relevant

BIOACCUMULATION

Bioconcentration factor (BCF): Octanol-water partition coefficient (LogKow):

TOXICITY

Chronic toxicity from studies: mg/l

1

Long-distance transport

Long-distance transport is not relevant for gaseous substances.

1

PMT/vPvM substances

i This criterion assesses whether a substance can pose a risk to drinking water supplies due to its persistence (P), its mobility (M), and its toxicity (T).

Information about PMT/vPvM properties

No evidence of PMT/ vPvM properties

1

Disruptions of the hormone system in the environment

i This indicator shows whether a substance can disrupt the hormone system of organisms in the environment.

Endocrine disrupting properties of the substance

No evidence of endocrine activity

R1234yf (2,3,3,3Tetrafluorpropen)

5

Environmental toxicity

3

 Aquatic toxicity

1

 PBT/vPvB substances and long-distance transport

5

 PMT/vPvM substances

1

 Disruptions of the hormone system in the environment

i The assessment of the environmental toxicity is based on the hazard statements entered at the beginning. In addition, additional sources can be taken into account for various aspects.

☐ This is an inorganic substance

3

Aquatic toxicity

i This criterion is used to assess the acute and chronic toxicity to aquatic organisms.

Relevant H statements H412

A The criterion is evaluated based on the classification. Entering additional information is possible but not required.

Acute aquatic toxicity (LC50) [mg/l]

Chronic aquatic toxicity (NOEC or EC10) [mg/l]

1

PBT/vPvB substances and long-distance transport

1

PBT/vPvB

Information on PBT properties

Own evaluation by entering measured values

PERSISTENCE

Simulation study: (not recorded) -- Days

Degradability: Not biodegradable

BIOACCUMULATION

Bioconcentration factor (BCF): Octanol-water partition coefficient (LogKow): 2.00

TOXICITY

Chronic toxicity from studies: 100.0000000 mg/l

1

Long-distance transport

Long-distance transport is not relevant for gaseous substances.

5

PMT/vPvM substances

i This criterion assesses whether a substance can pose a risk to drinking water supplies due to its persistence (P), its mobility (M), and its toxicity (T).

Information about PMT/vPvM properties

The substance is referred to in the literature as PMT/vPvM

1

Disruptions of the hormone system in the environment

i This indicator shows whether a substance can disrupt the hormone system of organisms in the environment.

Endocrine disrupting properties of the substance

No evidence of endocrine activity



3.5 Exposure potential

Propane

1

 Exposure potential for workers

-2

 Exposure potential for consumers

1

 Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Scenario for gas

Application quantities for gas

Evaluation

Results

Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	16	16	13	20	20
Worker / Inhalative	9	9	13	11	11
Consumer / Dermal		9		13	
Consumer / Inhalative		5		9	
Consumer / Orally		9		13	
Environment / Water	3	3	3	3	3
Environment / Air	5	5	5	5	5
Environment / Soil	3	3	3	3	3

R1234yf (2,3,3,3Tetrafluorpropen)

1

 Exposure potential for workers

-2

 Exposure potential for consumers

1

 Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Scenario for gas

Application quantities for gas

Evaluation

Results

Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	16	16	13	20	20
Worker / Inhalative	9	9	13	11	11
Consumer / Dermal		9		13	
Consumer / Inhalative		5		9	
Consumer / Orally		9		13	
Environment / Water	4	4	4	4	4
Environment / Air	5	5	5	5	5
Environment / Soil	4	4	4	4	4

The two gases are used in the same application. Therefore, the use scenarios are also the same.

For gases, compared to non-gaseous substances and mixtures, the assessment of exposure potentials is modified because it is assumed that relevant releases occur at exactly one point in the life cycle. For the current product, this happens at the end of life of the air conditioning system. Air conditioning systems are disposed of in a controlled manner, at least in Europe, and the coolant is collected largely emission-free. Therefore, only low emissions are expected.

Both gases are used as pure gases, so the highest concentration ranges are entered.

Since only small releases of refrigerants are to be expected, the possible exposure of both employees and the environment is rated as "low", i.e. green. Consumers do not normally come into contact with the coolants (blue colour).



3.6 Climate and ozone impacts

Propane

1

Climate and ozone

1

Intrinsic global warming potential

1

CO₂ emissions during production

1

Ozone-depleting effect

Intrinsic global warming potential

i Please enter the value of the global warming potential in the input field, if available. For some substances, the values are given in any case, (also) select the range in which the global warming potential lies. Only this value determines the rating for this criterion.

Global warming potential

3,00

Please select the range for the global warming potential.

Global warming potential less than 100

[Show comparison list](#)

CO₂ emissions during production

i Please enter the value for CO₂ emissions during production here and select the appropriate area from the options below. The evaluation is carried out according to your selection from the options. For a number of substances you find figures in the selection list.

Greenhouse gas emissions [kg CO₂ equivalents/kg substance]

0,54

Please select the range for aggregated greenhouse gas emissions as kg CO₂ equivalents/kg substance

< 1 kg CO₂-equivalent/kg substance

[Show comparison list](#)

Ozone-depleting effect

A An automatic comparison for H statement 420 and the problematic substance list 'Montreal Protocol' was carried out without result for the ozone depletion potential here and select the corresponding area from the options below. The evaluation is carried out according to your selection from the options. For a number of substances you find figures in the selection list.

Ozone Depletion Potential (ODP)

0,00000

Please select the range for ozone depletion potential.

ODP is 0

R1234yf (2,3,3,3Tetrafluorpropen)

3

Climate and ozone

1

Intrinsic global warming potential

5

CO₂ emissions during production

3

Ozone-depleting effect

Intrinsic global warming potential

i Please enter the value of the global warming potential in the input field, if available. For some substances, the values are given in any case, (also) select the range in which the global warming potential lies. Only this value determines the rating for this criterion.

Global warming potential

4,00

Please select the range for the global warming potential.

Global warming potential less than 100

[Show comparison list](#)

CO₂ emissions during production

i Please enter the value for CO₂ emissions during production here and select the appropriate area from the options below. The evaluation is carried out according to your selection from the options. For a number of substances you find figures in the selection list.

Greenhouse gas emissions [kg CO₂ equivalents/kg substance]

0,00

Please select the range for aggregated greenhouse gas emissions as kg CO₂ equivalents/kg substance

> 10 kg CO₂-equivalent/kg substance

[Show comparison list](#)

Ozone-depleting effect

A An automatic comparison for H statement 420 and the problematic substance list 'Montreal Protocol' was carried out without result for the ozone depletion potential here and select the corresponding area from the options below. The evaluation is carried out according to your selection from the options. For a number of substances you find figures in the selection list.

Ozone Depletion Potential (ODP)

0,00000

Please select the range for ozone depletion potential.

ODP greater than 0 and less than 0.02

R1234yf is used as a replacement for very ozone-damaging coolants. It has a relatively low GWP. However, its production is energy-intensive, thus associated with high CO₂ emissions (red). In addition, the production of R1234yf leads to the generation and emission of other ozone depleting



ChemSelect: Assessment of coolants (gases)

substances¹. Therefore, the ODP is set to yellow, even though R1234yf itself is not ozone-depleting. Since no specific value was found for these emissions, only the range is selected.

Propane is a component of natural gas and can be obtained relatively inexpensively. It has a low GWP, relatively little energy (CO₂ emissions) is used during production and it does not damage the ozone layer. Information on the lifecycle have been found on the internet.

3.7 Resource consumption

Propane

3

Resource consumption

1

Energy consumption

1

Water consumption

3

Consumption of raw materials

Energy consumption

Please enter the energy consumption for the production of 1 kg of substance here. Select the appropriate evaluation will be based on your selection of options. You can find the values for a selection of substance

Energy consumption [MJ/kg material]6,340

Energy consumption for the production of 1 kg of substance< 10 MJ / kg substance

[Show comparison list 'Energy consumption'](#)

Water consumption

Please enter the water consumption for the production of 1 kg of substance here. Select the appropriate evaluation will be based on your selection of options. For a number of substances you find figures in the

Water consumption [litres/kg substance]5,000

Water consumption for the production of 1 kg of substance< 5 litres / kg substance

[Show comparison list 'water consumption'](#)

Consumption of raw materials

When assessing raw material consumption, a distinction is first made between renewable raw material materials (e.g. metals). Both groups of raw materials can have problematic impacts on people and the have information about the origin of the raw materials.

☐ (not edited)
☐ The substance is made from RENEWABLE raw materials
☐ The substance is made from NON-RENEWABLE raw materials
☒ The substance is a product of petroleum or natural gas

R1234yf (2,3,3,3Tetrafluorpropen)

5

Resource consumption

5

Energy consumption

5

Water consumption

3

Consumption of raw materials

Energy consumption

Please enter the energy consumption for the production of 1 kg of substance here. Select the appropriate range fr will be based on your selection of options. You can find the values for a selection of substances in the comparison

Energy consumption [MJ/kg material]0,000

Energy consumption for the production of 1 kg of substance> 100 MJ /kg substance

[Show comparison list 'Energy consumption'](#)

Water consumption

Please enter the water consumption for the production of 1 kg of substance here. Select the appropriate area from be based on your selection of options. For a number of substances you find figures in the selection list.

Water consumption [litres/kg substance]0,000

Water consumption for the production of 1 kg of substance> 100 litres /kg material

[Show comparison list 'water consumption'](#)

Consumption of raw materials

When assessing raw material consumption, a distinction is first made between renewable raw materials (e.g. st materials (e.g. metals). Both groups of raw materials can have problematic impacts on people and the environm information about the origin of the raw materials.

☐ (not edited)
☐ The substance is made from RENEWABLE raw materials
☐ The substance is made from NON-RENEWABLE raw materials
☒ The substance is a product of petroleum or natural gas

¹ https://www.autoklimaanlage.info/fileadmin/user_upload/pdfs/Faktenblatt_1234yf_270812.pdf



ChemSelect: Assessment of coolants (gases)

With the exception of hydrofluoric acid, all fluorine-containing substances are rated red in the comparison list for energy consumption. Therefore R1234yf is also rated red. With the exception of aluminium fluoride, all fluorine-containing compounds are rated red in the comparison list for water consumption. Therefore, the water consumption of R1234 is also rated red. Both ratings are set to green for propane, which is viewed more as a “base material”. Here, information were available from a lifecycle inventory. Both compounds are made from petroleum or natural gas, so the assessment of raw material consumption does not differ.

3.8 Circularity potential

Propane	
1	Circularity
1	Potential for recovery
1	Potential to contaminate secondary materials

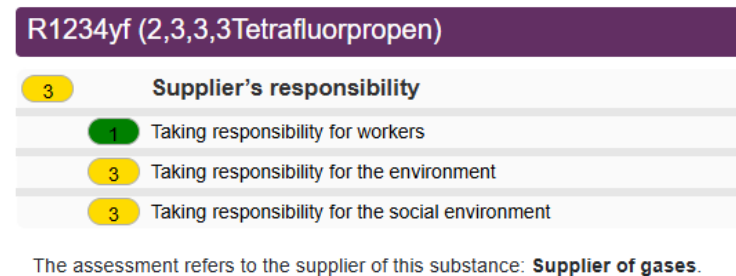
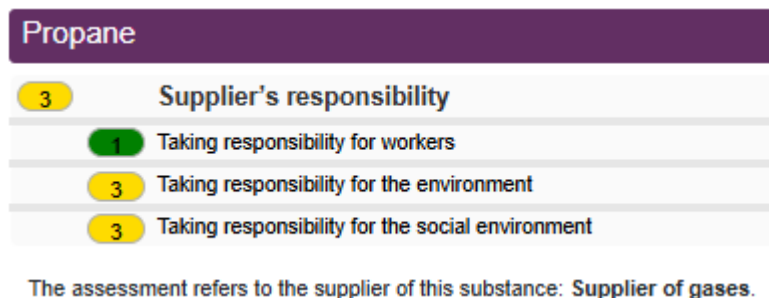
R1234yf (2,3,3,3Tetrafluorpropen)	
1	Circularity
1	Potential for recovery
1	Potential to contaminate secondary materials
 Time of gas release: Regulated disposal in waste treatment (The time of release is determined on the 'Exposure Potential' page)	

Both coolants can theoretically be recovered from the products in which they are used. Losses are possible along the lifetime from air conditioning systems but should be kept to a minimum (closed system). Contamination of the other components during the recycling stage is almost impossible due to the gaseous nature of the coolants. Therefore, the potential for recovery and the potential for contaminating secondary materials are both evaluated as green.

In Europe, products containing coolants are collected separately and sent for specific disposal. This may not be the case in other countries. It is up to the user whether this assessment should be changed as a result; the criterion only evaluates the potential, but not the actual disposal that takes place.



3.9 Supplier responsibility



Since both gases are purchased from the same supplier, the evaluation does not differ. The supplier's rating is shown in the figure below.

3.10 Summary

Propane

Aggregated presentation of substance evaluation

If criteria have not yet been worked on (colour grey), they are either evaluated as "realistic worst case - information need" (colour pink) in this summary or you are asked to work on the criterion in order to enable the evaluation.

Aspect: Particular concern
Mentioned on problem substance lists

Aspect: Indication of risks for health and environment
An exposure scenario for this substance is available.

Workplace	According to current knowledge, the substance is not considered dangerous. No relevant exposure is to be expected during the life cycle. Therefore, the risk potential is very low.
-2 Consumer	There is no exposure. Therefore the risk warning is not relevant.
Environment	According to current knowledge, the substance is not considered dangerous. No relevant exposure is to be expected during the life cycle. Therefore, the risk potential is very low.

Aspect: Life cycle impacts
Consideration of climate and ozone depletion, resource consumption and circularity.



ChemSelect: Assessment of coolants (gases)

R1234yf

Aggregated presentation of substance evaluation

ⓘ If criteria have not yet been worked on (colour grey), they are either evaluated as "realistic worst case - information needed" (colour pink) in this summary or you are asked to work on the criterion in order to enable the evaluation.

1 Aspect: Particular concern
Mentioned on problem substance lists

2 Aspect: Indication of risks for health and environment
An exposure scenario for this substance is available.

1 Workplace	According to current knowledge, the substance is not considered dangerous. No relevant exposure is to be expected during the life cycle. Therefore, the risk potential is very low.
5 Consumer	Although consumers do not come into direct contact with the substance (in the mixture), they may be exposed via the environment due to the substance's persistence. Therefore, the risk statement is red despite the lack of consumer use.
5 Environment	The substance has properties that are of particular concern. Even if only low levels of exposure are to be expected over the lifetime of the substance, the high level of concern means that there is a high risk potential.

3 Aspect: Life cycle impacts
Consideration of climate and ozone depletion, resource consumption and circularity.

Because of including the PMT/vPvM property of R1234yf's breakdown product TFA, also R1234yf itself is evaluated as a PMT in this example. For the risk indication, PMTs are considered as of very high concern for the environment and consumers. As a consequence, and according to EU risk assessment principles, any such exposure is evaluated as of concern (red). Consumers may be exposed via the environment, e.g. via drinking water. The environment is directly exposed and concentrations of persistent chemicals continuously build up. For workers, only exposures from the workplace are considered and hence, the PMT/vPvM properties do not play a role in the derivation of the risk indication.

The propane is not evaluated as hazardous to either human health or the environment, and hence the indication of risk is green for workers and the environment. It is "not relevant" for consumers, because no immediate contact occurs and – as propane is not persistent – the exposure of consumers is considered as "not relevant".

The life cycle impacts of R1234yf is evaluated as yellow mainly due to the high resource consumption and ozone depletion due to emissions of other, ozone depleting substances, during the production.



3.11 Substitution potential

R1234yf (2,3,3,3Tetrafluorpropen)

Calculation by average method

The evaluation has shown that the substance is not sustainable in key aspects. The following questions are intended to assess whether it is more likely that there are already less problematic alternatives (assessment green), i.e. whether substitution might be relatively easy and quick, or whether the replacement could be more complex, difficult and time-consuming (assessment red).

3 Potential for substitution

Please state your role

☐ (not edited) ☐ Formulators of mixtures ☒ Users of substances and/or mixtures

For what case would you like to evaluate the substitution potential? Potential to replace the substance as such ⓘ

1 - REPLACEMENT OF THE SUBSTANCE IN THE END USE

Availability of better alternatives?

Are alternatives available for the chemical Possibly, I have heard of better alternatives / found them in databases ⓘ

Is the application complex?

What is the end use of the substance Use as a process aid and/or to provide a service ▼

Requirements due to the conditions of use as **process aid** Increased stability against aggressive conditions ⓘ

Distribution/frequency of the function Common use ⓘ

Are there incentives for substitution through regulation?

Legal bans or restrictions encourage the development of alternatives.

Regulatory status of the substance/group of substances Substance/group of substances recently discussed as problematic ▼

The substitution potential of propane is not evaluated as no red result is displayed in the summary. Propane can be used as a replacement for R1234yf and therefore, the assessment of the substitution potential ends with selecting the option that alternatives are available.



4 Sustainability comparison

Sustainability comparison for substances		
Material	Propane	R1234yf (2,3,3,3Tetrafluorpropen)
Problem substance lists	1 Rank 1	1 Rank 1
Phys. chem. properties	5 Rank 2	3 Rank 1
Human toxicity	1 Rank 1	1 Rank 1
CMR	1 Rank 1	1 Rank 1
Skin/Eye	1 Rank 1	1 Rank 1
Endocrine	1 Rank 1	1 Rank 1
Other damage	1 Rank 1	1 Rank 1
Environmental toxicity	1 Rank 1	5 Rank 2
Aquatic Tox.	1 Rank 1	3 Rank 2
PBT/vPvB + Remote	1 Rank 1	1 Rank 1
PMT/vPvM	1 Rank 1	5 Rank 2
Endocrine	1 Rank 1	1 Rank 1
Exposure potential in workplaces	1 Rank 1	1 Rank 1
Exposure potential consumers	-2	-2
Exposure potential environment	1 Rank 1	1 Rank 1
Climate and ozone	1 Rank 1	3 Rank 2
Global warming potential	1 Rank 1	1 Rank 1
CO2 emissions	1 Rank 1	5 Rank 2
Ozone depletion	1 Rank 1	3 Rank 2
Resource consumption	3 Rank 1	5 Rank 2
Energy	1 Rank 1	5 Rank 2
Water	1 Rank 1	5 Rank 2
Raw materials	3 Rank 1	3 Rank 1
Circularity	1 Rank 1	1 Rank 1
Recovery	1 Rank 1	1 Rank 1
Pollution	1 Rank 1	1 Rank 1
Supplier's responsibility	3 Rank 1	3 Rank 1
Worker	1 Rank 1	1 Rank 1
Environment	3 Rank 1	3 Rank 1
Social environment	3 Rank 1	3 Rank 1

When comparing the two substances, it is obvious that R1234yf is rated red more often than propane. In addition, a central criterion, environmental toxicity, is rated red, which has a particularly high weight. It must be noted, that this is due to including TFA, a degradation product of R1234yf in the assessment. As no possibilities exist to include information about classification proposals, it was decided not to include this in the assessment, but to wait for the official decision.

Among the criteria relating to chemical safety, propane only has a red rating for PC properties. This suggests that propane is a good alternative to R1234yf from a sustainability perspective. ChemSelect cannot assess the technical feasibility.



5 Additional assessment aspects

In this example, the fact that the refrigerant R1234yf breaks down to trifluoro acetic acid (TFA) was considered in the assessment by attributing its hazardous properties to the parent compound R1234yf for the environment, while only keeping it in mind for human health due to a lack of respective opportunities to enter uncertainties in classification. In order to remain simple, and as many downstream users of chemicals lack respective information, ChemSelect does not foresee or ask for the assessment of breakdown products but the assessment focuses on the substances as used. However, if information is available on e.g. the ecotoxicity and toxicity of breakdown products can be considered, as shown in the example. It is good to document this explicitly.

The ozone depletion potential (ODP) of R1234yf was also entered into the tool by not only considering the substance as such, but also emissions from the production process. During research on R1234yf's (ODP), the information about emissions of substances that do harm the ozone layer during the production of R1234yf was found by coincidence. As these emissions are most likely related to halogenated compounds (fluorine-containing ones), it can be assumed that not similar emissions would occur for propane.

The assessment of exposure potentials is different for gases than it is for non-gaseous substances as normally, the release of gases mainly happen during one specific life stage and the exposure main exposure pathways are inhalation (humans) and air (environment). This is due to the fact that either the release is intended (at a specific stage) or the release is not intended and hence occurs during the waste stage. As gases are hard to contain, significant release normally does not spread over several lifecycle stages, allowing for an assessment short-cut where only the one relevant lifecycle stage is identified.

6 Conclusions

R1234yf performs better than propane when it comes to PC properties, because it is non-flammable. However, there is a higher environmental toxicity due to its degradation product TFA; and possibly also due to a future classification as reprotoxic, in the human toxicity criterion. This is generally considered to be more relevant for the sustainability assessment than the PC properties, as the latter are predominantly relevant in the workplace and frequently can be controlled with risk management measures.

The exposure potential does not differ for the gases since the application situation is unchanged.

In terms of environmental impact, R1234yf performs worse than propane, although there is only an estimate for CO₂ emissions in production based on the comparison lists, but no data from databases. In addition, the formation of ozone-depleting substances during the production of R1234yf was taken into account when assessing ozone depletion. The ODP of the substance itself is "0", i.e. without this consideration it would also be rated green.

Although not present as a separate feature, ChemSelect users can account for the degradation and intermediates of chemicals (in this case, the degradation of R1234yf to trifluoroacetic acid), if they implicitly include the properties of degradation products in the assessment of the parent compound / precursor. In this example, this is central to the overall evaluation.