

Category E 'C5 non-cyclics' - Chemical Category Justification

(NB : all compositions are in w/w for liquids and v/v for gases)

Category definition and its members	
1.1.	Category Definition
1.1.a.	Category Hypothesis
<p>The C5 non-cyclics category covers hydrocarbon streams that are predominantly derived from the ethylene process and other associated C5 processes. Imported streams will need to confirm that they meet the chemical description and are in domain. These hydrocarbon streams have a carbon number distribution that is typically C3 – C7. All of the streams in this category contain significant levels of non-cyclic mono- and di-olefins and more than 1% isoprene. Companies importing streams will need to confirm that such streams meet the chemical description and are in domain.</p> <p>It is reasonable to assume that the phys-chem and environmental fate properties of the category members will be very similar due to the small spread of carbon numbers. Environmental effects will behave in a similar manner, acting via narcosis. With regard to mammalian endpoints, category members are volatile liquids with inhalation and skin contact representing the primary routes of exposure. CNS depression, (marker substance: isopentene) and irreversible effects (the latter linked to the presence of isoprene) are likely to drive health hazard assessment. It can therefore be assumed that streams meeting the applicability domain will behave in a similar manner and that the use of read-across is valid.</p> <p>For mammalian endpoints, the classification of these streams will be driven by the content of isoprene, which is greater than 1% for all category members.</p>	
1.1.b.	Applicability domain (AD) of the category
<p>The category applies to streams with the following PIONA* analysis: > 20% (iso)paraffins, olefins and/or naphthenics and > 20% olefins with more than 1% isoprene and a carbon number distribution which will centre on 5 with a predominant range of 3 – 7.</p> <p><i>Boiling Point – the streams in this category will boil predominantly in the range of 0 - 75°C</i></p> <p>Specific components (The range entered below is that currently based on received analytical data, it is not intended to be prescriptive. See section 1.3).</p> <p><i>Isoprene : > 1%</i></p> <p><i>Pentane : up to 30%</i></p> <p><i>Benzene: <0.1 – 0.9%</i></p> <p><i>Toluene: <0.1 – 4%</i></p> <p><i>1,3-butadiene - <0.1% to 3%</i></p> <p>PIONA* :</p> <p>(Iso)Paraffins – up to 75% : C# 3 - 7</p> <p>Olefins – up to 99% : C# 3 - 7</p> <p>Naphthenics – up to 30%</p> <p>Aromatics – up to 5%</p> <p><i>*: PIONA refers to a description of the type of hydrocarbons present, paraffins, isoparaffins, olefins, naphthenics and aromatics. It does not refer to a specific type of analysis or determination.</i></p>	
1.2.	Category Members

CAS Number	CAS Description	Registered Substance Name
68476-43-7	Hydrocarbons, C4-6, C5-rich	Hydrocarbons, C4-6, C5-rich
		C5 Olefins
68476-55-1	Hydrocarbons, C5-rich	Crude C5 Stream
68477-35-0	Distillates (petroleum), C3-6, piperylene-rich	Distillates (petroleum), C3-6, piperylene-rich
		Piperylene
		Piperylene cut
91995-41-4	Distillates (petroleum), heat-soaked steam-cracked naphtha, C5-rich	Piperylene

1.3. Purity / Impurities

The substances in this category are UVCBs and as such are considered to be 100% pure. The term impurity is not relevant for UVCBs, however, substances will be described using the following:

- Known constituents present at 10% or greater (if any), identified by IUPAC name and EC number/CAS number, indicating typical concentrations and/or concentration ranges;
- Constituents relevant for hazard classification (if any);
- Constituents relevant for PBT assessment (if any).

Primary marker

Isoprene (CAS# 78-79-5): tox classification: Carc Cat 2 R45, Mut Cat 3 R68

Tox statements:

Isoprene is regulated as a carcinogen in the EU following evidence in experimental animals.

2. Category justification

C5 non-cyclics is a UCVB category and therefore identification of trends between category members is not appropriate. The data across the C5 non-cyclics category is reasonably homogenous. The majority of the boiling points are reported as being between 0 and 75°C which means that all category members are volatile liquids which will be expected to have similar partitioning in the environment and therefore similar potential for exposure. With respect to environmental effects, the hydrocarbons in these streams will all act via narcosis. The data are also reasonably homogenous with respect to carbon number, though not to hydrocarbon class. The data available on the category members indicates that isoprene is present in the streams at >1% which compared to the other hydrocarbons in the streams will be the major driver for the human health assessment.

3. Data matrix

C5 non-cyclics is a UCVB category and therefore identification of trends between category members is not appropriate and therefore, according to the ECHA Guidance on information requirements and chemical assessment Chapter R.6, it is not feasible to establish a full data matrix for this category. Consequently, a data set that applies to all members of this category has been developed.

4. Conclusions per endpoint for C&L, PBT/vPvB and dose descriptor

CLASSIFICATION AND LABELLING

Physico-chemical Hazard Assessment

- **Boiling point** - The measured boiling point of streams in this category is in the range 25°C to 60°C. The agreed category boiling range is 0 to 75°C.
- **Partition coefficient** - The partition coefficients for streams in this category range from log Kow 2.2-5, with the majority of components having a log Kow in the range 3.1-3.9.
- **Flash point** - The flash point of streams in this category is <-30°C.

flashpoint <23°C and initial boiling point ≤35°C.

Flam. Liquid 1 (Hazard statement: H224: Extremely flammable liquid and vapour.).

flashpoint >23°C and initial boiling point ≥35°C.

Flam. Liquid 2 (Hazard statement: H225: Highly Flammable liquid and vapour.)

Human Health Hazard Assessment

- **Toxicokinetics** – The marker substances, in their pure form, have well-defined toxicokinetic parameters that have been taken into account during the derivation of their respective DNEL's. The overall DNEL of this category is driven by the DNEL for isoprene.
- **Acute toxicity** – Based on percentages of the component substances 2-methylbut-2-ene, cyclopentene, and cyclopentadiene /3a,4,7,7a-tetrahydro-4,7-methanoindene (DCPD) all streams should be classified as harmful via oral and dermal exposure. Streams with >9% DCPD (or cyclopentadiene) should also be classified for acute inhalation toxicity. Data for a number of component substances show that dizziness and sleepiness are experienced at air levels <20 mg/L. In addition C5 non-cyclics streams also warrant classification as an aspiration hazard on the basis of kinematic viscosity.
- **Irritation** – C5 non cyclics streams and a number of component and marker substances are irritating to the skin, eyes and respiratory tract.
- **Sensitisation** – C5 non-cyclics streams are not expected to be dermal or respiratory sensitisers on the basis of data for component and marker substances.
- **Repeat dose toxicity** – A major finding in repeat dose studies with C5 non-cyclics streams and major components is male rat-specific kidney change which is considered not to be relevant to humans. As all streams within this category contain less than 1% benzene and less than 10% toluene no classification is required for this endpoint.
- **Genetic toxicity** – Although studies with C5 non-cyclics streams showed no evidence of genotoxicity, there are substantial data on the genotoxicity of a number of specific components present in some streams. Of these, benzene, isoprene and 1,3-butadiene have been shown to be mutagenic in vivo. As isoprene, a Category 3 mutagen, is present in all streams at a concentration of 1% or more and 1,3-butadiene or benzene, both category 2 mutagens, are present in some streams at concentrations of ≥0.1% C5 non-cyclics streams are considered to be mutagenic in vivo.
- **Carcinogenicity** – There are no specific carcinogenicity data on any of the streams within this category. However, there are substantial data on the carcinogenicity of several components present in some streams. Of these, benzene, isoprene and 1,3-butadiene have been shown to be carcinogenic. As isoprene is a Category 2 carcinogen and is present in all streams at a concentration of 1% or

greater and 1,3-butadiene or benzene are Category 1 carcinogens and present in some streams at concentrations of 0.1% or more then C5 non-cyclics streams are considered to be carcinogens.

- **Toxic to reproduction** –It is recognised that there are data gaps for both developmental toxicity study and multi-generation studies. as C5 non-cyclics streams contain at least 1% isoprene, which is classified as a Cat 3 mutagen and a Cat 2 carcinogen under EU/DSD and appropriate risk management measures are implemented (handled in controlled conditions). Available data on C5 non cyclics streams and component and marker substances are sufficient for classification and labelling purposes. For streams that contain toluene at concentrations greater than or equal to 5% (EU/DPD) or 3% (GHS/CLP), classification is required for developmental toxicity.

Environmental Hazard Assessment

- **Biodegradation** - The streams in this category are not considered to be readily biodegradable.
- **Bioaccumulation** - Log BCF have been calculated for various representative components of these streams. The calculated values range from 1.2-2.1.
- **Ecotoxicity** - Results are based both on nominal loading rates (WAF) and mean measured concentrations. Data reported is based on WAF, which better represent the potential toxicity of the test substance. Algae were found to be less sensitive than either invertebrates or fish which had similar sensitivity to the test substance (EL50 6.96 mg/l WAF and LL50 14.1 mg/l WAF respectively).

Based on the results of the hazard assessment the streams in this category are classified as: Aquatic Chronic 2 (Hazard statement: H411: Toxic to aquatic life with long lasting effects).

CONCLUSION FOR PBT

The screening assessment of the available data indicates that the properties of the members of this category do not meet the specific criteria detailed in Annex XIII or do not allow a direct comparison with all the criteria in Annex XIII but nevertheless indicate that the substance would not have these properties and therefore are not considered PBT/vPvB.

CONCLUSION FOR DOSE DESCRIPTOR

Environment

Deriving PNECs for UVCB substances based on WAF information is inappropriate. As the substance is a hydrocarbon UVCB the hydrocarbon block method has been used for environmental risk assessment (see REACH guidance, R7, app.13-1). The Petrorisk model (Redman, A. (2010). PETRORISK Users Guide, HydroQual, Inc., for Conservation of Clean Air and Water in Europe (CONCAWE)), was used for the environmental assessment. Blocks of C5-C6 carbon atoms and with a boiling point range of 34.5°C to 110.6°C were used in the modelling exercise. The model assigns individual structures from the library to the hydrocarbon blocks that the user enters. The input parameters are provided in Appendix B of the CSR. Details of the library structure mapping, some relevant physico-chemical properties and the mass fraction that is assigned to each chemical are also found in this appendix.

Health

Risk characterization will be based on the premise that a marker substance with a low DN(M)EL present at high concentration in a stream will possess a greater relative hazard potential than a marker substance with a higher DN(M)EL present at the same or lower concentration.

In the case of this stream, the hazardous marker substances present are ranked as follows:

Marker substance	Indicative concentration (%)	Inhalation		Dermal	
		DN(M)EL mg/m ³	Relative hazard potential (max % ÷ DN(M)EL)	DN(M)EL mg/kg bwt/d	Relative hazard potential (max % ÷ DN(M)EL)
Isoprene	≤25	8.4	3.0	23.7	1.05
1,3-Butadiene	≤3	2.21	0.90	na[h]	na
Benzene	≤0.9	3.25	0.28	23.4	<0.01
Toluene	≤4	192	0.02	384	0.01

Based on this analysis, demonstration of “safe use” for occupational hazards associated with the presence of 25% isoprene will also provide adequate protection against hazards arising from benzene, 1,3-butadiene and toluene that are also present.

The long-term inhalation and dermal DNELs for isoprene will therefore be used for worker risk characterization.