

Category C 'C4, low 1,3-butadiene (<0.1%)' - 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 'C4, low 1,3-butadiene (<0.1%)' category covers hydrocarbon streams containing high purity hydrocarbons, hydrocarbon substances with impurities and complex hydrocarbon reaction products. These hydrocarbon streams have a carbon number distribution that is predominantly C4 with a range from C3-C5 and less than 0.1% 1,3-butadiene. Category members are typically produced from the steam-cracking of naphtha and following the extraction of 1,3-butadiene from a C4-rich stream. 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. The streams will have similar environmental effects as their constituents cover a narrow carbon range and all act in similar manner, via narcosis. With regard to mammalian endpoints, category members are very volatile low boiling liquids, liquefied gases or gases with inhalation representing the primary route of exposure. There are no significant drivers for health effects as the major substances - butenes are simple asphyxiant and long-term irreversible effects are not anticipated. It can therefore be assumed that streams meeting the applicability domain will behave in a similar manner and therefore the use of read-across is valid.</p> <p>As the 1,3-butadiene content of the streams is less than 0.1% w/w (or v/v for gases) for all category members they will not be impacted by any classification or hazard assessment based on butadiene as a constituent.</p>		
1.1.b.	Applicability domain (AD) of the category	
<p>The category applies to streams with essentially the following PIONA* analysis: 100% (iso)paraffins and olefins with less than 0.1% 1,3-butadiene and a predominant carbon number distribution of 3 – 5</p> <p>Boiling Point –the streams in this category will boil predominantly in the range of -15 - +15°C</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>1,3-butadiene - <0.1%</i></p> <p>PIONA* :</p> <p>(Iso)Paraffins – up to 100% : C# 3 - 5</p> <p>Olefins – up to 90% : C# 3 - 5</p> <p>Naphthenics – typically <1%</p> <p>Aromatics – typically <1%</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

91052-98-1	Hydrocarbons, C4, 1,3-butadiene-free	Hydrocarbons, C4, 1,3-butadiene-free
92045-23-3	Hydrocarbons, C4, steam-cracker distillate	Hydrocarbons, C4, steam-cracker distillate
95465-89-7	Hydrocarbons, C4, 1,3-butadiene- and isobutene-free	hydrocarbons C4, <0.1% 1,3-butadiene, isobutene-free
95465-90-0	Hydrocarbons, C4, n-butene conc.	Hydrocarbons, C4, n-butene conc.
95465-91-1	Hydrocarbons, C4, butane conc., n-butene-contg.	Hydrocarbons, C4, butane conc., n-butene-contg.

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).

2. Category justification

The '**C4, low 1,3-butadiene (<0.1%)**' category covers hydrocarbon streams containing high purity hydrocarbons, hydrocarbon substances with impurities and complex hydrocarbon reaction products. These hydrocarbon streams have a carbon number distribution that is predominantly C4 with a range from C3-C5 and less than 0.1% 1,3-butadiene. Category members are typically produced from the steam-cracking of naphtha and following the extraction of 1,3-butadiene from a C4-rich stream. The physico-chemical properties associated with these types of UVCBs indicated that they comprise a category based on the range of boiling points (from -15°C to 15°C) and will have similar behaviour in the environment. The log Kow ranges from >2.31 to 2.4 and the streams in this category are considered to be readily biodegradable. The mammalian toxicity information and environmental assessment also indicated that the streams in this category exert similar effects.

3. Data matrix

'**C4, low 1,3-butadiene (<0.1%)**' 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 ranged from -11.73°C to 3.71°C (agreed category boiling point range of -15°C to 15°C).
- **Partition coefficient** - The streams in this category have partition coefficients ranges from log

Kow 2.31 to 3.4.

- **Flash point** - The flash point of streams in this category does not need to be conducted as members of this category are gases at room temperature. Some streams will have the following classification.

Flashpoint of < 23 °C and initial boiling point ≤ 35 °C.

Flam. Gas 1 (Hazard statement: H220: Extremely flammable gas.)

Human Health Hazard Assessment

- **Toxicokinetics** – There are no specific studies on the streams in the C4, low 1,3-butadiene category (CAS Numbers; 91052-98-1, 92045-23-3, 95465-89-7, 95465-90-0 and 95465-91-1) but data are available on the component substances albeit in pure form. The overall DNEL for this category is driven by the component substance 2-methylpropene. Metabolism and distribution studies on 2-methylpropene show that metabolic elimination was first order and that metabolism was saturable in both rats and mice and was blocked by inhibitors of P450 enzymes. In rats, there was rapid metabolism to oxidised metabolites (isobutenediol and 2-hydroxyisobutyric acid) which were excreted in urine. Studies using in vitro rat, mouse and human liver systems demonstrated that the lowest rates of biotransformation to the epoxide metabolite were found in human liver, followed by rat then mouse
- **Acute toxicity** – Members of the C4 low 1,3-butadiene category are flammable gases at room temperature and therefore the requirement for data on acute oral and dermal toxicity is waived in accordance with REACH Annex XI. There are no specific studies on the streams in this category (CAS Numbers; 91052-98-1, 92045-23-3, 95465-89-7, 95465-90-0 and 95465-91-1) but data on the component substances (butane, isobutane and butene isomers) indicate that the acute inhalational toxicity of this category is low. The LC50 values for all substances are in excess of 10,000 ppm (22,948 mg/m³) and butane and isobutane are considered to be Generally Recognised as Safe and may be used in food products.
- **Irritation** – Members of the C4 low 1,3-butadiene category are flammable gases at room temperature and therefore the requirement for data on skin and eye irritation is waived in accordance with REACH Annexes VII and VIII (column 2 adaptation). All members of this category are gases, and liquid gases may cause burns and frostbite due to the extreme cold of the liquid.
- **Sensitisation** – Not sensitising.
- **Repeat dose toxicity** – Members of the C4 low 1,3-butadiene category are flammable gases at room temperature and therefore the requirement for data on oral and dermal repeat dose toxicity is waived in accordance with REACH Annex XI. There are no specific studies on the streams in this category (CAS Numbers; 91052-98-1, 92045-23-3, 95465-89-7, 95465-90-0 and 95465-91-1) but data on the component substances (butane, isobutane and butene isomers) indicate that members of this category have low sub-chronic toxicity. Inhalation exposure is the most relevant route. No significant exposure-related toxicological effects or target organ toxicity have been observed in inhalation studies in rats or mice for 6 weeks (butane and isobutane) or up to 2 years (butene isomers). Nasal lesions were observed in 2 year rodent studies on 2-methylpropene at the highest concentration and the NOAEC of 2000 ppm (4589 mg/m³) in rats is based on the lack of effect at this concentration.
- **Genetic toxicity** – The available data therefore indicates that members of this category are not likely to be mutagenic in humans.

- **Carcinogenicity** – There are sufficient data available on component substances to conclude that streams within the C4 low 1,3-butadiene category have a low potential for human carcinogenicity.
- **Toxic to reproduction** – There are data-gaps for reproduction and developmental toxicity studies but in accordance with section 1 of REACH Annex XI, testing does not appear to be scientifically necessary since data are available on component substances which are adequate for the purposes of classification and labelling and/or risk assessment of the UVCB substances included in this category. No biologically significant treatment-related reproductive toxicity or effects on reproductive endpoints in repeat dosing studies were observed in rats or mice after inhalational exposure to butane, isobutane, 1-butene, 2-butene and 2-methylpropene. A developmental toxicity study conducted in rats on 2-methylpropene (butene isomer) produced no treatment-related developmental toxicity. It is concluded that streams within the C4 low 1,3-butadiene category are not toxic to reproduction and have no effect on fertility or development

Environmental Hazard Assessment

- **Biodegradation** - Results from all predictions using BOWIN showed the substances except isobutane to be readily biodegradable. Isobutane, although not readily biodegradable was shown to biodegrade. Therefore streams within this Category are expected to degrade rapidly.
- **Bioaccumulation** - the bioaccumulation in aquatic species study does not need to be conducted as these streams have a low potential for bioaccumulation (components have a log octanol water partition coefficient less than 3).
- **Ecotoxicity** – CAS Numbers 92045-23-3 and 95465-89-7 are both listed in Annex I but are not classified for environmental hazards. Additionally constituent substances, butane, isobutane, butene, isobutene are listed in Annex 1 but are not classified for environmental hazards. This Category would not be classified for environmental hazards

Based on the available data streams in this category are classifiable for environmental 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: Members of this category are not classified for human health or the environment, are not a CMR and are not PBT or vPvB. Therefore derivation of PNECs is not required.

Human Health:

Members of this category are not classified for human health or the environment, are not a CMR and are not PBT or vPvB. Therefore derivation of DNELs is not required.