

Category J 'low benzene naphthas' - 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 low benzene naphthas category contains hydrocarbons (aliphatic, aromatic and olefinic) with carbon numbers predominantly in the C5-C12 range and boiling from 30C to 300C. Members of this category contain <0.1% benzene and contain varying amounts of toluene, xylenes and n-hexane. Some category members contain PAHs, where this is the case anthracene has been quantified. Category members are typically produced by the distillation of products from a steam cracking process or by pyrolysis. Companies importing streams will need to confirm that such streams meet the chemical description and are in domain.</p> <p>By definition, from the category, these streams have overlapping hydrocarbon compositions, within a defined range, and hence, will have similar properties. It is therefore reasonable to assume that the components of the category will behave in a reasonably predictable manner, and with respect to phys-chem and environmental fate and effect properties read-across is valid.</p> <p>With regard to mammalian endpoints, category members are liquids with inhalation the major route of potential exposure. The primary health effect by inhalation is likely to be irritation after short term high exposure with potential for CNS effects. No significant health effects are anticipated from longer term exposures, other than those driven by toluene which is present in some streams.</p>		
1.1.b.	Applicability domain (AD) of the category	
<p>The category applies to streams with the following PIONA* analysis: predominantly (Iso)Paraffins, olefins, naphthenics and aromatics and less than 0.1% benzene and a carbon number range of predominantly 5-12.</p> <p><i>Boiling Point – the streams in this category will boil predominantly in the range of 30 - 300°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>Benzene: <0.1%</i></p> <p><i>Toluene: up to 50%</i></p> <p><i>1,3-butadiene: <0.1%</i></p> <p><i>Anthracene : up to 0.2% (streams with this component at >0.1% are candidates for authorisation as anthracene is a confirmed PBT)</i></p> <p>PIONA* :</p> <p>(iso)Paraffins – up to 5% : C# 5 - 12</p> <p>Olefins – up to 70% : C# 5 - 12</p> <p>Naphthenics – up to 10% : C# 5 - 12</p> <p>Aromatics – up to 100% : C# 5 – 12</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
101316-66-9	Hydrocarbons, C6-8, hydrogenated sorption-dearomatized, raffination toluene	Hydrocarbons, C6-8, hydrogenated sorption-dearomatized, toluene raffination.

64741-98-6	Extracts (petroleum), heavy naphtha solvent	Extracts (petroleum), heavy naphtha solvents
64742-94-5	Solvent naphtha (petroleum), heavy arom.	Solvent naphtha (petroleum), heavy arom.
68476-55-1	Hydrocarbons, C5-rich	Hydrocarbons, C5-rich
68477-39-4	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C8-10 fraction	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C8-10 fraction
68516-20-1	Naphtha (petroleum), steam-cracked middle arom.	Naphtha (petroleum), steam-cracked middle arom.

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);
- Toluene, present at up to 50%, is a developmental toxicant and classification is driven by the levels of toluene present in the stream.

2. Category justification

The **low benzene naphthas** category contains hydrocarbons (aliphatic, aromatic and olefinic) with carbon numbers predominantly in the C5-C12 range. Category members are typically produced by the distillation of products from a steam cracking process or by pyrolysis. Members of this category contain <0.1% benzene and contain varying amounts of toluene, xylenes and n-hexane. Some category members contain PAHs, where this is the case anthracene has been quantified. The physico-chemical properties associated with these types of UVCBs indicated that they comprise a category based on the range of boiling points (from 30°C to 300°C) and will have similar behaviour in the environment. The log Kow ranges from 2.8 to >6.5 and the streams in this category are not 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

Low benzene naphthas 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 boiling point of streams in this category is in the range of 25°C to 332°C and a category range used for assessment was agreed to be 30°C to 300°C.
- **Partition coefficient** - The partition coefficient of streams in this category is in the range 2.8 to >6.5.
- **Flash point** - The flash point of streams in this category is in the range -30°C to 77°C at 1013 hPa.

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 ≥60°C.

Flam. Liquid 3 (Hazard statement: H226: Flammable liquid and vapour.)

Human Health Hazard Assessment

- **Toxicokinetics** – The key marker substance for this category is toluene and the toxicokinetic parameters for toluene have been taken into account in the DNEL proposals.
- **Acute toxicity** –Low benzene naphtha streams are of low acute toxicity by the oral, dermal and inhalation routes and do not warrant classification for these end-points. However streams that contain ≥20 % toluene should be classified as vapours may cause drowsiness. In addition low benzene naphtha streams also warrant classification as an aspiration hazard on the basis of kinematic viscosity.
- **Irritation** – Low benzene naphtha streams and toluene are irritating to the skin.
- **Sensitisation** – Low benzene naphthas and toluene are not skin or respiratory sensitisers.
- **Repeat dose toxicity** –Subacute exposure to a low benzene naphtha streams by inhalation, and a related stream by dermal application did not indicate any specific target organ toxicity which would warrant classification. However, there are substantial data on the repeated dose toxicity of toluene which demonstrates significant target organ toxicity and, when present at concentrations greater than or equal to 10%, this component substance will influence classification due to repeat dose mammalian toxicity effects.
- **Genetic toxicity** –. Low benzene naphtha streams and toluene are not genotoxic.
- **Carcinogenicity** – There are no specific carcinogenicity data on any of the streams within this category but low benzene naphtha streams are not genotoxic. Toluene is not classified as a carcinogen.
- **Toxic to reproduction** –It is recognised that there are data gaps for both developmental toxicity study and multi-generation studies. Available data on one stream and on toluene 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 have not been shown to be readily biodegradable and will not be considered readily biodegradable.
- **Bioaccumulation** - The calculated BCF of representative components of the streams range from 99 to 5790.
- **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-C12 carbon atoms and with a boiling point range of 30 °C to 300 °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.

Human 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. It will also focus on the potential of the markers to cause serious long-term health effects rather than on short-term or irritation-related effects.

Against this background, the most hazardous marker substances present in these streams are highlighted in the following table:

Workers

Marker substance	Indicative concentration (%)	Inhalation		Dermal	
		DN(M) ELmg/m ³	Relative hazard potential(max % ÷ DN(M) EL)	DN(M) ELmg/kg bwt/d	Relative hazard potential(max % ÷ DN(M) EL)
benzene	< 0.1	3.25	<0.031	23.4	0.004
toluene	≤50	192	0.260	384	0.13
1,3-butadiene	< 0.1	2.21	<0.045	na ¹	na ¹
anthracene	≤0.2	<i>low systemic toxicity, no DNELs required</i>			

Based on this analysis, demonstration of “safe use” for inhalation and dermal hazards associated with the presence of up to 50% toluene will also provide adequate protection against inhalation hazards arising from the other marker substance present.

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

General population

Against this background, the most hazardous marker substances present in these streams are highlighted in the following table (details of the DN(M) EL derivations follow this table):

Marker	Indicative	Inhalation	Dermal	Oral
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substance	concentration(%)	DN(M) ELmg/m ³	Relative hazard potential(m ax % ÷ DN(M) EL)	DN(M) ELmg/kg bwt/d	Relative hazard potential(max % ÷ DN(M) EL)	DN(M) ELmg/kg bwt/d	Relative hazard potential(m ax % ÷ DN(M) EL)
General population							
benzene	< 0.1	<i>supply of steams containing ≥ 0.1% benzene prohibited</i>					
toluene	≤ 50	56.5	0.88	226	0.22	8.13	6.15
1,3-butadiene	< 0.1	<i>supply of steams containing ≥ 0.1% butadiene prohibited</i>					
anthracene	≤ 0.2	<i>low systemic toxicity, no DNELs required</i>					

Demonstration of “safe use” for inhalation, dermal and oral hazards associated with the presence of 50% toluene will also provide adequate protection against any hazards arising from other components also present.

The long term inhalation, dermal and oral DNELs for toluene will therefore be used for general population risk characterization.