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| **Committee of Experts on the Transport of Dangerous Goods  and on the Globally Harmonized System of Classification and Labelling of Chemicals 25 June 2021** |
| **Sub-Committee of Experts on the Transport of Dangerous Goods**  **Fifty-eighth session**  Geneva, 28 June-2 July 2021 Item 3 of the provisional agenda  **Listing, classification and packing** |

Classification of UN 1010, mixtures of Butadienes and Hydrocarbons – vapour pressure and density

Submitted by the European Chemical Industry Council (Cefic)

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| **Executive Summary:**  This document gives explanatory information on the vapour pressure (at 70 °C) and density (at 50 °C) of butadienes/hydrocarbon-mixtures with 20% (or more) 1,3-butadiene.  **Action to be taken: -**  **Related documents:** ST/SG/AC.10/C.3/2021/22 (Cefic) |

Introduction

1. In working document ST/SG/AC.10/C.3/2021/22 from Cefic it is stated, under 2. (c), that “these mixtures [butadiene/hydrocarbon mixtures with 20-40 % butadiene] all have a vapour pressure at 70 °C not exceeding 1.1 MPa (11 bar) and a density at 50 °C not lower than 0.525 kg/l.”

2. This statement is based upon a theoretical approach using data from the following publication: *Redeker/Schön - 6. Nachtrag zu Sicherheitstechnische Kennzahlen brennbarer Gase und Dämpfe, Tabelle H, 1990. ISBN 3-8064-9936-5*.

3. In the above-mentioned publication the following data on vapour pressure (in MPa) at 70 °C (MPa) and density (in kg/l) at 50 °C is listed.

vapour pressure at 70 °C density at 50 °C

C3 hydrocarbon gases

Propylene (UN 1077) 3.04 0.459

Propane (UN 1978) 2.58 0.45

C4 hydrocarbon gases

Isobutane (UN 1969) 1.08 0.518

Isobutylene (UN 1055) 0.98 0.554

Butylene-1 (UN 1012) 0.96 0.558

1,3-Butadiene (UN 1010) 0.92 0.582

Butane (UN 1011) 0.79 0.543

trans-2-Butylene (UN 1012) 0.79 0.567

cis-2-Buylene (UN 1012) 0.73 0.584

4. The “most volatile and lightest” C4 hydrocarbon gas with a vapour pressure (VP) near 1.1 MPa and density near 0.525 kg/l is by far isobutane - it’s VP is just below 11 bar and it’s density is below 0.525 kg/l.

5. For a ‘worst case’ approach, to calculate the maximum possible vapour pressure and the minimum possible density, we can take a mixture of 20 % butadiene, 1 % propylene (as impurity – although C3 hydrocarbon gases under normal conditions should be absent) and 79 % isobutane (in practise this will not be the case as the main component in these mixtures next to butadiene is isobutylene). Nevertheless, our worst case still delivers a vapour pressure below 1.1 MPa (1.068) and a density above 0.525 kg/l (0.530).

Mixture for max VP partial pressure partial density

Isobutane 79% 0.853 0.409

1,3-Butadiene 20% 0.184 0.116

Propylene 1% 0.030 0.005

Total 100% vapour pressure density

1.068 0.530

6. Based upon this calculation it can be concluded that all relevant mixtures have a vapour pressure below 1.1 MPa at 70 °C and a density above 0.525 kg/l at 50 °C.

7. The database of AspenHYSY lists a vapour pressure of Isobutane at 70 °C of 1.088 MPa and the database of Conval of 1.086 MPa. 1,3-Butadiene has a vapour pressure of 0.915 MPa at 70 °C.

8. Using these databases gives vapour pressures at 70 °C of 1.073 or 1.071 MPa. Both also well below 1.1 MPa.