

**Committee of Experts on the Transport of Dangerous Goods
and on the Globally Harmonized System of Classification
and Labelling of Chemicals**

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Sub-Committee of Experts on the Transport of Dangerous Goods

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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)

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

- 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.”
- 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.*
- 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-Butylene (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 - its VP is just below 11 bar and its 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.