How to bring your registration dossier in compliance with REACH – Tips and Hints Part 4

Vapour Pressure

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Vapour Pressure

A key property for assessing some toxicological and environmental hazards. The vapour pressure indicates if the substance will be available for inhalation and allows the determination of the volatility of a substance from an aqueous medium or soil. Moreover, it is important for physical hazard assessment.

Vapour Pressure (REACH Annex VII, 7.5)

"The saturation pressure above a solid or a liquid substance at constant temperature"

It is recommended to determine the vapour pressure for at least two temperatures, for volatile substances preferably at 20 and 50 ºC.

Test methods:

- Method A.4 of Regulation (EC) No 440/2008
- OECD Test Guideline 104

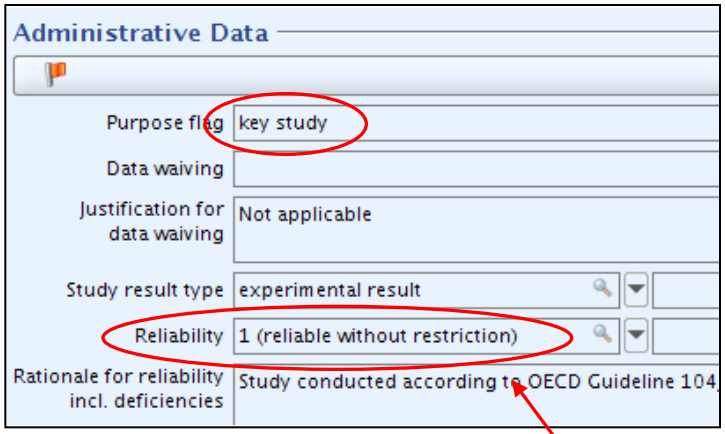
Measuring Methods

Measuring Method	Substances		Estimated Repeatability (1)	Estimated Reproducibility (1)	Recommended Range	Existing Standard
	solid	liquid				
1.4.1. Dynamic method	Low melting	yes	Up to 25 %	Up to 25 %	10^3 Pa to 2 × 10^3 Pa	—
			1 to 5 %	1 to 5 %	2 × 10^3 Pa to 10^5 Pa	—
1.4.2. Static method	yes	yes	5 to 10 %	5 to 10 %	10 Pa to 10^5 Pa (2)	NFT 20-048 (5)
1.4.3. Isoteniscope	yes	yes	5 to 10 %	5 to 10 %	10^2 Pa to 10^5 Pa	ASTM-D 2879-86
1.4.4. Effusion method Vap. Pres.balance	yes	yes	5 to 20 %	5 to 50 %	10^{-3} Pa to 1 Pa	NFT 20-047(6)
1.4.5. Effusion method weigt loss	yes	yes	10 to 30 %	—	10^{-3} Pa to 1 Pa	—
1.4.6. Gas saturation method	yes	yes	10 to 30 %	Up to 50 %	10^{-4} Pa to 1 Pa (2)	—
1.4.7. Spinning rotor method	yes	yes	10 to 20 %	—	10^{-4} Pa to 0,5 Pa	—

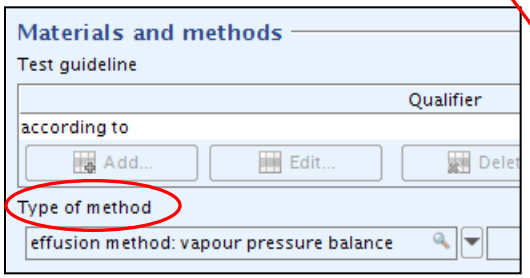
Each method has an applicability range!

Vapour Pressure reporting in IUCLID

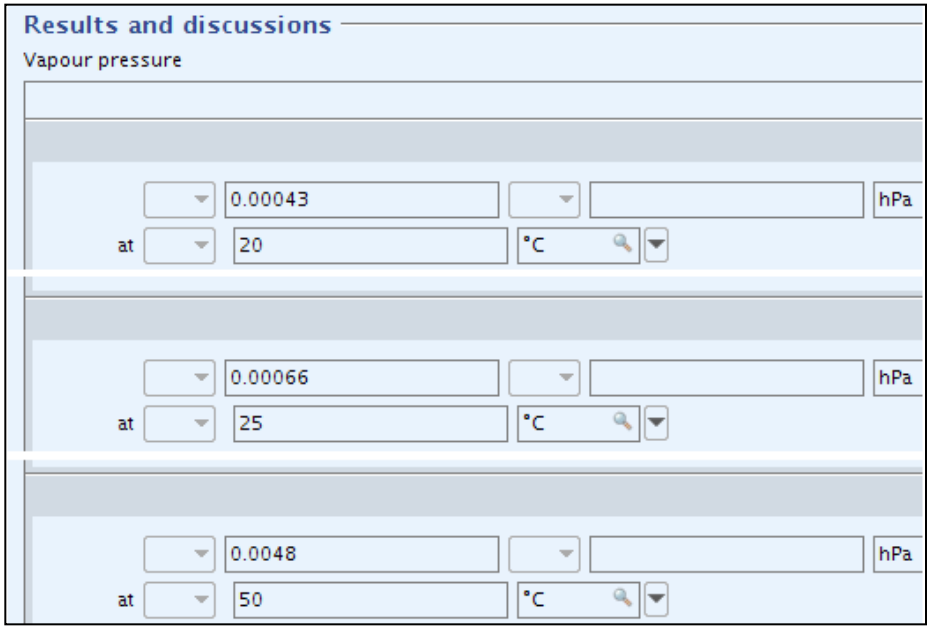
Endpoint study record: for an experimental study the purpose flag is *key study*



Type of method used



The Vapour pressure results are reported (in Pa) for at least two temperatures:



The reliability must be adequate for the endpoint to be considered fulfilled!!

Adaptation possibilities: REACH

	Column 1 Standard Information Required	Column 2 Specific Rules for Adaptation from Column 1
Annex VII	7.5 Vapour pressure	The study does not need to be conducted if the melting point is above 300 °C. If the melting point is between 200 and 300 °C, a limit value based on measurement or a recognised calculation method is sufficient.

Guidance, Chapter R.7a, section R.7.1.5.1:

Further adaptation possibilities

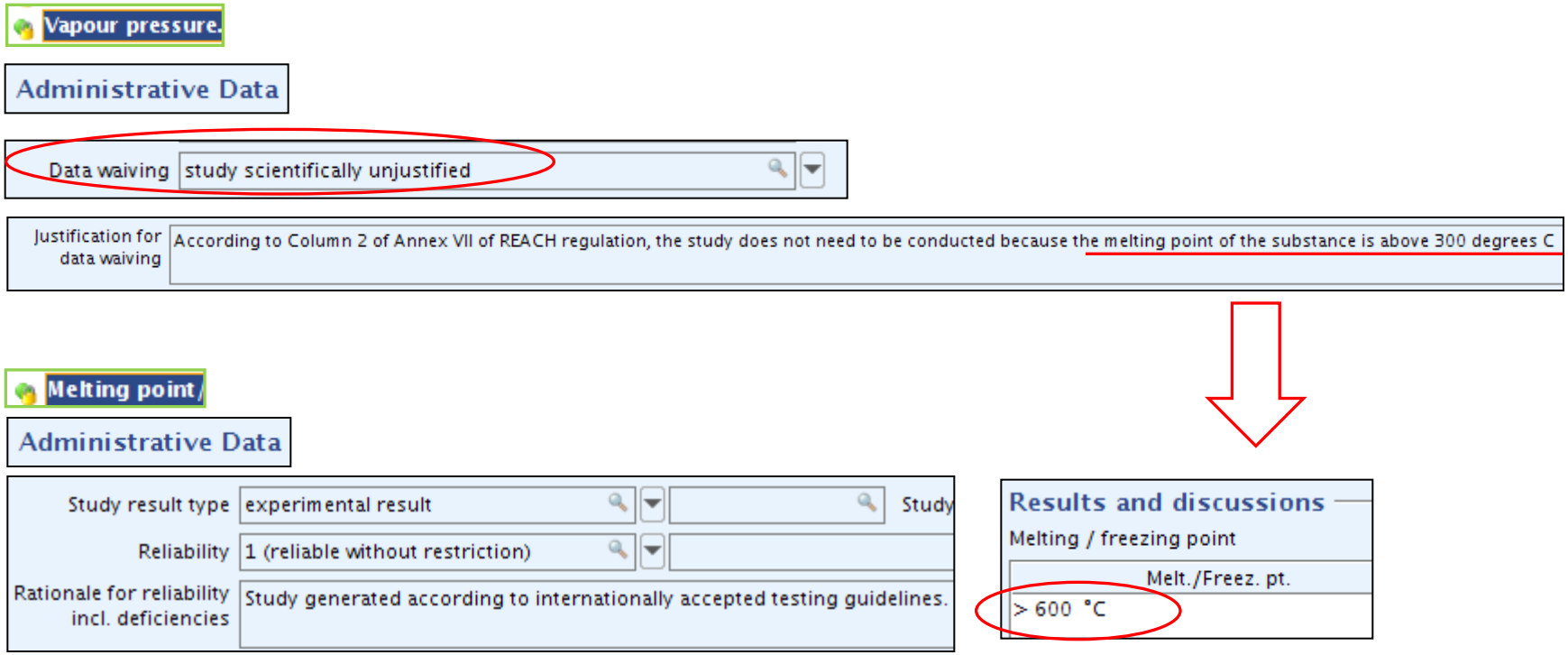
Vapour pressure testing is also not required for chemicals with a standard boiling point of <30 ºC, as these substances will have a vapour pressure above the limit of measurement (i.e. 10^5 Pa).

Annex XI: other adaptation possibilities

- Testing is technically not possible:
  - for substances which decompose during measurement or which are unstable or explosive
  - for self-reactive, pyrophoric or corrosive substances
- (Q)SARs
  - determination by experiment is not possible
- Weight of Evidence
  - several independent sources of existing data

Example: adaptation possibility of the standard information requirements

Adaptation possibility according to column 2 of Annex VII to REACH



Other adaptation possibilities: (Q)SAR

- Results from a (Q)SAR may be used when the conditions in Annex XI, Section 1.3 are met

- QMRF and QPRF have to be included in the relevant endpoint study record:
  - (Q)SAR Model Reporting Format: describes the applied (Q)SAR model
  - (Q)SAR Prediction Reporting Format: describes how the estimate was derived from the application of the model to a specific substance

(Q)SAR reporting in IUCLID

Vapour pressure.

Administrative Data

Study result type	estimated by calculation
Reliability	2 (reliable with restrictions)

Study result type	(Q)SAR
Reliability	2 (reliable with restrictions)

Data source

Reference type	Author	Year	Title	Bibliographic source
other: QSAR model	University of Georgia, Karickhoff SW et al	2007	SPARC online calculator, release x4.0.1264-s4.0.1263	http://sparc.chem.uga.edu/sparc

Overall remarks, attachments

Attached background material

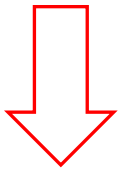
Attached document	
QMRF Vapour Pressure 20100611.pdf / 238.94 KB (application/octet-stream)	QMRF
QSAR Prediction Reporting Format VP 919-30-2 20100611.pdf / 26.15 KB (application/octet-stream)	QPRF

ECHA Practical guide 5: How to report (Q)SARs
http://echa.europa.eu/documents/10162/13655/pg_report_qsars_en.pdf

Guidance document on QSARs and grouping (R.6)
http://echa.europa.eu/documents/10162/13632/information_requirements_r6_en.pdf

Estimation method

- It is reported in Appendix of test methods (EU A.4 and OECD 104) and it can be used:
  - in deciding which experimental method to use
  - in providing an estimate when an experimental method cannot be applied
  - in identifying cases where an experimental measurement can be omitted since the vapour pressure is likely to be < 10-5 Pa



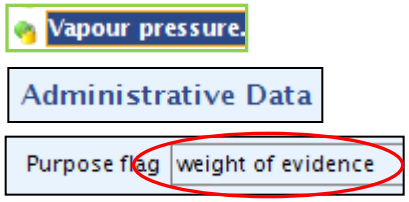
- If the results of the estimation method indicate a vapour pressure >10-5 Pa, you may still be requested to conduct an experimental study

Other adaptation possibilities: Weight-of-evidence

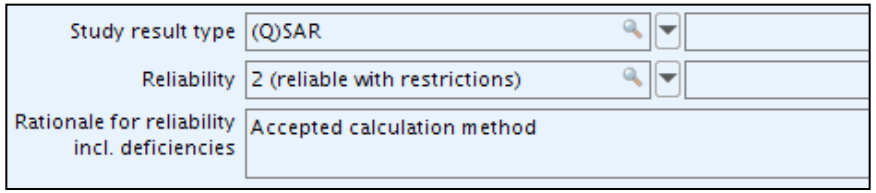
- More than one independent source of existing data (study report, (Q)SAR, literature data) not sufficiently reliable alone
- It entails an assessment of the independent available information in showing that the endpoint is fulfilled and a key value selected
- In practical terms this means:
  - each single source of information in a separate endpoint study record
  - the conclusions from the available information in the endpoint study summary

Weight-of-evidence: example

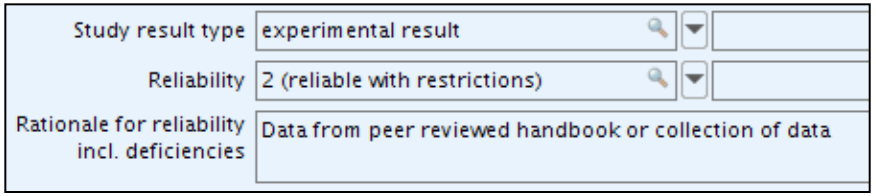
Endpoint study records



1)

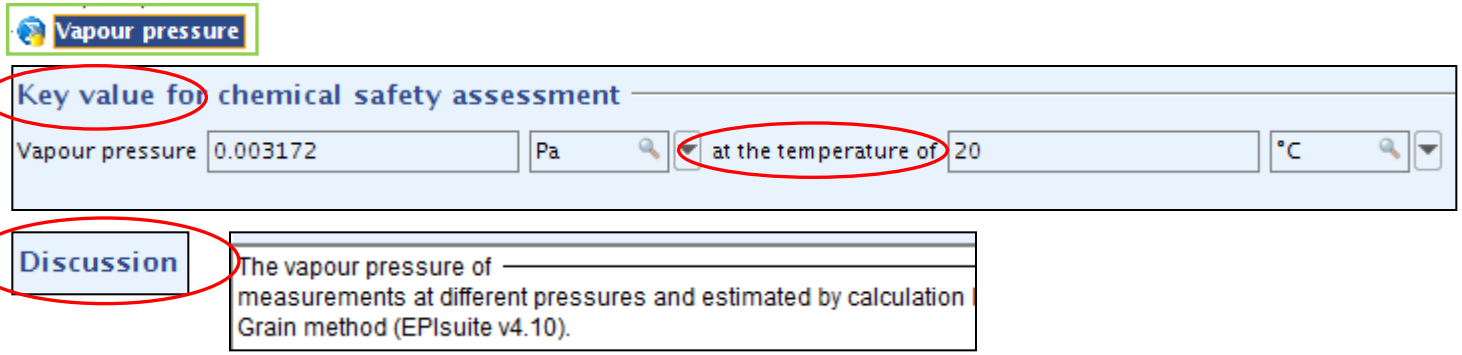


2)



The two sources must be independent!

Endpoint study summary:



ECHA Practical guide 2: How to report weight of evidence
http://echa.europa.eu/documents/10162/13655/pg_report_weight_of_evidence_en.pdf
Guidance document on evaluation of available information (R.4)
http://echa.europa.eu/documents/10162/13643/information_requirements_r4_en.pdf

When applying adaptation possibilities

- Annex XI: the conditions must be met
  - 1.2. WoE: at least two independent sources of existing data; conclusions on the property
  - 1.3. (Q)SAR: QMRF, QPRF attached
  - 2. Testing technically not possible: description

- REACH, column 2 of Annex VII: melting point > 300 ºC to be shown

- Guidance R.7A: boiling point < 30 ºC to be proven

Vapour pressure: recommendations

- It is important to describe clearly which adaptation possibility was used
- It is always necessary to include an explanation on the scientific reasoning applied
- Clearly demonstrate the reasons for each adaptation
- When this is not possible, the result of an experimental study has to be provided

Thank you!

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