

Impacts and uses of physico-chemical data under REACH

Tests	Impact on other physico-chemical tests	Impact on toxicology	Impact on risk assessment and risk management
Melting/freezing point	Choice of method for flash point, flammability, autoflammability, oxidising properties, explosive properties. If decomposition occurs during the melting point study, a boiling point does not need to be measured.		Indicator for the physical state of a compound.
Boiling point	Related to vapour pressure. Affects classification as "highly flammable" or "extremely flammable".		Indicator for the physical state of a compound. Consider process temperature for risk assessment.
Relative density	Used in the determination of viscosity.		Fire-fighting measures: H ₂ O extinguishers may not be suitable if $D_{4}^{20} < 1$.
Vapour pressure	When handling a substance with high vapour pressure, care should be taken to minimise vapour losses during tests. Related to boiling point. May influence the ability to measure an accurate log K_{ow} .	Choice of: – dermal or inhalation exposure route for acute toxicity test; – route of exposure for sub-acute toxicity test; – exposure and excretion routes for toxicokinetic assessment. The vapour pressure enables a statement about inhalative absorption in the living organism.	Human health risk assessment. Vapour pressure is a key parameter in determining environmental fate and behaviour. Determination of atmospheric behaviour as for exposure of man via the environment calculations.
Surface tension	May influence the approach for testing log K_{ow} . Can occasionally interfere with measurement of water solubility.	Surface active substances have a higher local irritant or corrosive effect. As a consequence of local corrosion, the dermal uptake of a substance can be enhanced.	Environmental fate.
Water solubility	Surface tension test not applicable for water solubility < 1 mg/l at 20 °C. Need to prepare 90% saturated solution (up to a maximum of 1 g/l) for surface tension test. Time to achieve saturation can be relevant to solution preparation for surface tension test. Water solubility affects concentration used in hydrolysis test. May influence the ability to measure an accurate log K_{ow} .	Impact on toxicokinetic behaviour.	Environmental classification and labelling. Water solubility is a key parameter in determining environmental fate and behaviour.
Partition coefficient n-octanol/water (K_{ow})	Generally, substances with a high log K_{ow} will be hydrophobic and have low water solubilities. Substances with negative log K_{ow} will be hydrophilic and have high water solubilities.	Toxicokinetic behaviour: K_{ow} indicates the potential for absorption across biological membranes and for passive diffusion (e. g. prediction of dermal absorption). It provides information on the potential for accumulation in the body. Choice of suitable vehicle for toxicity studies.	Environmental classification and labelling. Log K_{ow} is a key parameter in determining environmental fate and behaviour and is used as a surrogate for bioaccumulation potential in the absence of bioaccumulation tests.
Granulometry		Computation of inhalable, thoracic and respirable fractions as a function of size of particles.	
Dissociation constant	The process of dissociation (depending on pH) in solution can have a huge effect on water solubility, K_{ow} , and volatilisation of a substance.	Exposure to hydrolysis products <i>in vivo</i> : the dissociation constant indicates the potential for absorption from the gastrointestinal tract, because ionised compounds are thought not to cross biological membranes.	The dissociation constant is a key parameter in determining environmental fate and behaviour.
Viscosity	Choice of methods for the determination of density.	Parameter for aspiration hazard.	Assessment of spreadability of liquids.