

ProtoPHYSICHEM

ProtoPHYSICHEM is a computational (*in silico*) tool focused on the prediction of endpoints related with the physicochemical properties of chemical substances.

ProtoPHYSICHEM mainly includes, but is not limited to, endpoints used by REACH, a European Union regulation, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry.

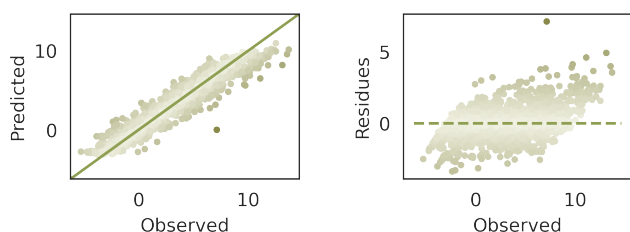
Endpoint

Physical-chemical properties: Vapour pressure.

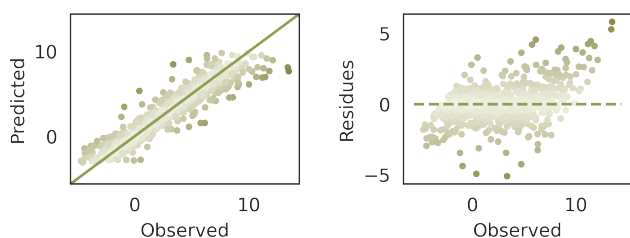
The vapour pressure of a substance is defined as the saturation pressure above a solid or a liquid substance at constant temperature. At the thermodynamic equilibrium, the vapour pressure of a pure substance is a function of temperature only.

Metrics

Training set



Validation set



| Parameters | Training | Validation |
|---------------------------|----------|------------|
| R ² score | 0.92 | 0.90 |
| Mean absolute error (MAE) | 0.70 | 0.82 |
| Mean squared error (MSE) | 0.97 | 1.39 |
| Median absolute error | 0.49 | 0.55 |
| Explained variance | 0.92 | 0.90 |