

API-Surrogate search: Data curation

3.2. Calculated properties:

- ✓ Certain properties like molecular formula, number of rotatable bonds, TPSA, etc. can be calculated using RDKit module.
- ✓ List of APIs and their experimental properties

3.3. Experimental properties

- Current version of app have experimental properties for melting point, enthalpy of fusion, pKa, Peff, solubility, and LogD.
- The experimental data for these properties was either downloaded, fetched, scraped, or cleaned from different public sources /repositories.