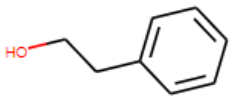
Propersea

Structure-based predictions at the Physical Sciences Data-science Service

What does Propersea do?

Propersea is an online structure-based prediction engine for physicochemical properties and IUPAC naming.



OCCc1ccccc1 [?]

$C_8H_{10}O$

Molar Mass: 122.2 g·mol^{-1}

IUPAC Name [?]: 2-phenylethanol

Propersea allows the user to:

- Predict **physicochemical properties**, including:

Melting point
Boiling point
Density
logP
Solubility
Viscosity
Polarizability
Molar refractivity
Polar surface area
pK_a
H-bond acc/don
Ionization energy

- Predict the **IUPAC name** from a structure, SMILES or InChI

	Value	95% Credible Interval [?]		Reliability [?]
Melting Point [?]	-3.13 °C	-24.2	18.0	High
Boiling Point [?]	220.0 °C	211.0	226.0	High
Flash Point [?]	97.3 °C	89.0	105.0	High
Density [?]	1.04 g·cm^{-3}	1.02	1.06	High
Solubility (@ 25 °C) [?]	29.0 g·L^{-1}	12.0	59.0	High
Viscosity (@ 25 °C) [?]	7.5 mPa·s	5.0	11.0	Medium
Surface Tension (@ 25 °C) [?]	39.0 dynes·cm^{-1}	38.0	40.0	Medium
logP [?]	1.5	1.3	1.8	High
logK_{OA} [?]	6.0	5.5	6.4	Medium
Refractive Index [?]	1.54	1.49	1.6	High
Molar Refractivity [?]	37.2 cm^3·mol^{-1}	–	–	–
Polarizability [?]	14.8 Å^3	–	–	–
Polar Surface Area [?]	20.2 Å^2	–	–	–
Dipole Moment [?]	1.92 D	–	–	–
pK_a (atom 10) [?]	14.9	–	–	–
H-bond Acceptors [?]	1.0	–	–	–
H-bond Donors [?]	1.0	–	–	–
Rotatable Bonds [?]	2.0	–	–	–
Heat of Formation [?]	-131.0 kJ·mol^{-1}	–	–	–
Ionization Energy [?]	9.54 EV	–	–	–

Example of results from Propersea

Access Propersea via the Physical Sciences Data-science Service

at www.psds.ac.uk email: info@psds.ac.uk

Propersea Structure-based predictions

How does Propersea work?

Predictions are made based on chemical structures entered by:

- **Structure search** via the ChemDoodle® structure drawing interface
- Typing or pasting a **SMILES string** or **InChI** (including InChI=)

The properties are predicted through a variety of algorithms, including:

- RDKit algorithms
- Semi-empirical quantum methods
- Fragment/ atom contribution calculations
- Bayesian Additive Regression Trees
- Transformer neural networks

The predicted value is returned in the results interface. For those properties predicted using the Bayesian algorithms it also returns an interval for the 95% confidence, along with a measure of how well the molecule compares to molecules contained in the training set.
If a property prediction is deemed non-sensical due to the predicted phase, the property may be omitted from results.

Limitations of Propersea

Propersea performs best for organic compounds and performance on inorganics, orgometallics and inorganic-organic mixtures is known to be lower.

Reliability metrics for these compounds would show as 'Low' or 'Very Low'.

How do I access Propersea?

Propersea is provided to the UK academic community via the **PSDS at www.psds.ac.uk**. The Physical Sciences Data-science Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **www.psds.ac.uk**. If working off-campus, a PSDS username and password will be issued.

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