

1-Octanol
111-87-5 | DTXSID7021940

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.76e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.04e-01

Confidence level: 8.72e-01

Nearest Neighbors from the Training Set

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Heptylamine

Measured: 7.94e-02

Predicted: 2.73

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Dodecanoic acid

Measured: 2.27e-02

Predicted: 7.83e-05

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Hexanedinitrile

Measured: 2.16e-01

Predicted: 1.98e-03

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Triethylene glycol

Measured: 8.51e-03

Predicted: 8.10e-04

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Succinimide

Measured: 2.42e-01

Predicted: 2.34e-04