

1-Hexanol
111-27-3 | DTXSID8021931

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.10

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

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cis-Nanophine

Measured: 5.01

Predicted: 6.12

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Piperidine, 1-methyl-

Measured: 4.47

Predicted: 5.88

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Quinoline

Measured: 3.80

Predicted: 6.66

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Aniline

Measured: 1.62

Predicted: 3.43