

1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-
376-18-1 | DTXSID3059923

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.04e-15 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.79e-01

Confidence level: 4.85e-01

Nearest Neighbors from the Training Set

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Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-

Measured: 7.20e-15

Predicted: 1.32e-14

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

Measured: 1.12e-13

Predicted: 6.54e-14

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Propane, 1,1,1,2,2,3,3-heptafluoro-3-methoxy-

Measured: 1.18e-14

Predicted: 1.85e-14

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HFE-347pcf2

Measured: 9.40e-14

Predicted: 6.55e-14

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Perfluorotributylamine

Measured: 6.00e-17

Predicted: 1.14e-16