

1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-
2043-47-2 | DTXSID1062122

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: 6.27e-14 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.32e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

Image not found

HFE-347pcf2

Measured: 9.40e-14

Predicted: 6.55e-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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Flurothyl

Measured: 1.63e-13

Predicted: 1.12e-13

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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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Sevoflurane

Measured: 7.30e-14

Predicted: 4.40e-14