

1-Butanol, 2,2,3,3,4,4,4-heptafluoro-
375-01-9 | DTXSID4059914

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: 6.54e-14 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.46e-01

Confidence level: 6.83e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 1.12e-13

Predicted: 6.54e-14

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HFE-347pcf2

Measured: 9.40e-14

Predicted: 6.55e-14

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Heptafluoroisopropyl methyl ether

Measured: 1.52e-14

Predicted: 2.77e-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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1-Propanol, 2,2,3,3,3-pentafluoro-

Measured: 9.29e-14

Predicted: 6.57e-14