

PFOA

335-67-1 | DTXSID8031865

Model Performance

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: 6.97e-01

Global applicability domain: Outside

Local applicability domain index: 1.87e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

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4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

Measured: 1.11

Predicted: 8.08e-01

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2-Amino-1-naphthalenesulfonic acid

Measured: 0.78

Predicted: 8.06e-01

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1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 0.4

Predicted: 3.80e-01

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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

Measured: 0.48

Predicted: 7.40e-01

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Sodium 3-nitrobenzenesulfonate

Measured: 0.7

Predicted: 7.21e-01