

1,2,4,5-Tetrachlorobenzene
95-94-3 | DTXSID7024320

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.64e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.39e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

Image not found

1,2,4,5-Tetramethylbenzene

Measured: 5.40e-03

Predicted: 1.01

Image not found

Docosane

Measured: 5.53e-02

Predicted: 4.97e-06

Image not found

Silane, tetraethyl-

Measured: 3.90e-02

Predicted: 7.80

Image not found

Isoquinoline

Measured: 4.60e-01

Predicted: 2.62e-02

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Phthalide

Measured: 2.10e-01

Predicted: 2.25e-03