

Cyclosarin
329-99-7 | DTXSID00861875

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.81

Global applicability domain: Inside

Local applicability domain index: 3.75e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

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Sulfolane

Measured: 7.08

Predicted: 6.91

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Benzenesulfonamide

Measured: 4.79

Predicted: 2.10

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o-Toluenesulfonamide

Measured: 2.57

Predicted: 2.00

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1,5-Naphthalenediamine

Measured: 4.47

Predicted: 3.93

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1,8-Naphthalenediamine

Measured: 6.31

Predicted: 3.19