

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -8.27 °C

Global applicability domain: Inside

Local applicability domain index: 4.44e-01

Confidence level: 3.23e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclosarin

Measured: -30.0

Predicted: -8.27

[Image not found](#)

Diglycidyl resorcinol ether

Measured: 42.5

Predicted: 66.1

[Image not found](#)

Pinacolyl
methylphosphonofluoridate

Measured: -42.0

Predicted: -48.2