

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 216 °C

Global applicability domain: Inside

Local applicability domain index: 6.40e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

Image not found

Cyclosarin

Measured: 239

Predicted: 216

Image not found

Triethyl phosphate

Measured: 216

Predicted: 211

Image not found

Phosphonic acid, vinyl-, diethyl ester

Measured: 202

Predicted: 205

Image not found

Diisopropyl fluorophosphate

Measured: 183

Predicted: 195

Image not found

Diethyl ethylphosphonate

Measured: 198

Predicted: 196