

Phosphonic acid, vinyl-, diethyl ester
682-30-4 | DTXSID70218372

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.31 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diisopropyl methylphosphonate

Measured: 8.88e-01

Predicted: 4.69e-01

[Image not found](#)

Triethyl phosphate

Measured: 2.74

Predicted: 1.41

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Dimethyl propyl phosphate

Measured: 2.97

Predicted: 2.43

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Phosphoric acid, diethyl propyl ester

Measured: 2.55

Predicted: 6.52e-01