

Erythritol
149-32-6 | DTXSID6043919

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.38e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.09e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found

Diethylene glycol

Measured: 3.00e-11

Predicted: 2.21e-11

Image not found

1,2-Propylene glycol

Measured: 1.20e-11

Predicted: 1.34e-11

Image not found

2-(2-Ethoxyethoxy)ethanol

Measured: 5.72e-11

Predicted: 3.59e-11

Image not found

1-Methoxy-2-propanol

Measured: 1.86e-11

Predicted: 1.93e-11

Image not found

Bis(2-methoxyethyl) ether

Measured: 1.75e-11

Predicted: 1.96e-11