

Butyl nitrate
928-45-0 | DTXSID70239143

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: 1.60e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.17e-01

Confidence level: 8.13e-01

Nearest Neighbors from the Training Set

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Butyl nitrate

Measured: 1.71e-12

Predicted: 1.60e-12

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Isobutyl nitrate

Measured: 9.20e-13

Predicted: 1.33e-12

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Amyl nitrate

Measured: 3.14e-12

Predicted: 2.43e-12

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n-Propyl nitrate

Measured: 7.30e-13

Predicted: 8.54e-13