

Tris(2-hydroxyethyl) isocyanurate
839-90-7 | DTXSID4026266

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 5.25e-12 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.09e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

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Isoproturon

Measured: 1.20e-11

Predicted: 3.23e-11

Image not found

Cycloate

Measured: 3.54e-11

Predicted: 2.98e-11

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Diethyl sulfate

Measured: 1.80e-12

Predicted: 1.55e-12

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

Image not found

Propylene dinitrate

Measured: 3.20e-13

Predicted: 3.59e-13