

Famotidine
76824-35-6 | DTXSID5023039

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.42

Global applicability domain: Outside

Local applicability domain index: 2.00e-01

Confidence level: 6.89e-01

Nearest Neighbors from the Training Set

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Tris(2-hydroxyethyl) isocyanurate

Measured: 1.58

Predicted: 1.61

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Melamine

Measured: 3.80

Predicted: 2.45

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Pentaerythritol

Measured: 1.26

Predicted: 1.25

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Triisopropanolamine

Measured: 5.75e-01

Predicted: 7.42e-01

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Malaoxon

Measured: 1.12

Predicted: 1.49