

Thiamine disulfide
67-16-3 | DTXSID6046890

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: 3.31

Global applicability domain: Outside

Local applicability domain index: 1.51e-01

Confidence level: 7.00e-01

Nearest Neighbors from the Training Set

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N,N,N',N',N",N"-
Hexakis(methoxymethyl)-1,3,5-
triazine-2,4,6-triamine

Measured: 3.47

Predicted: 4.50

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Tris(2-butoxyethyl) phosphate

Measured: 5.75

Predicted: 6.32

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Malaoxon

Measured: 1.12

Predicted: 1.49

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Docusate sodium

Measured: 9.33

Predicted: 8.95

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Tris(2-hydroxyethyl) isocyanurate

Measured: 1.58

Predicted: 1.61