

Thioacetamide
62-55-5 | DTXSID9021340

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.18

Global applicability domain: Inside

Local applicability domain index: 9.68e-01

Confidence level: 6.82e-01

Nearest Neighbors from the Training Set

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Butylamine

Measured: 3.61

Predicted: 4.09

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Isopentyl alcohol

Measured: 4.52

Predicted: 4.24

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Pyrrolidine

Measured: 4.07

Predicted: 4.10

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1-Butanol

Measured: 4.19

Predicted: 4.03

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1-Pentanol

Measured: 4.69

Predicted: 4.17