

N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine
3089-11-0 | DTXSID9027520

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.52

Global applicability domain: Outside

Local applicability domain index: 2.31e-01

Confidence level: 5.47e-01

Nearest Neighbors from the Training Set

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Ethanol, 2-((4,6-bis(dimethylamino)-s-triazin-2-yl)methylamino)-

Measured: 1.96

Predicted: 2.19

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Hexamethylmelamine

Measured: 2.73

Predicted: 2.28

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NSC298112

Measured: 3.45

Predicted: 2.95

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Trimelamol

Measured: 0.4

Predicted: 9.99e-01