

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

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 145 °C

Global applicability domain: Outside

Local applicability domain index: 2.24e-01

Confidence level: 3.43e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Azaserine

Measured: 154

Predicted: 176

[Image not found](#)

Dyphylline

Measured: 162

Predicted: 161

[Image not found](#)

HC Blue 2

Measured: 95.5

Predicted: 111

[Image not found](#)

2',3'-Dideoxycytidine

Measured: 218

Predicted: 209

[Image not found](#)

Nicorandil

Measured: 92.5

Predicted: 115