

Propanedioic acid, diethyl-
510-20-3 | DTXSID9060150

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.85e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 3.29e-01

Nearest Neighbors from the Training Set

Image not found

Piperidine

Measured: 2.87e-06

Predicted: 26.2

Image not found

Pentan-2-ol

Measured: 3.14e-06

Predicted: 5.03

Image not found

Dimethoxymethane

Measured: 1.91e-07

Predicted: 170

Image not found

Piperazine

Measured: 9.00e-08

Predicted: 7.31e-01

Image not found

1,2,3,4-Tetrachlorobenzene

Measured: 2.25e-06

Predicted: 3.76e-02