

Isobutylmalonic acid
4361-06-2 | DTXSID60195885

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: 6.47e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 3.64e-01

Nearest Neighbors from the Training Set

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Piperidine

Measured: 2.87e-06

Predicted: 26.2

Image not found

Dimethoxymethane

Measured: 1.91e-07

Predicted: 170

Image not found

Pentan-2-ol

Measured: 3.14e-06

Predicted: 5.03

Image not found

Piperazine

Measured: 9.00e-08

Predicted: 7.31e-01

Image not found

Cycloheptanone

Measured: 2.88e-07

Predicted: 1.00