

Endothal
145-73-3 | DTXSID7024081

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: 160 °C

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

Image not found

Endothal

Measured: 144

Predicted: 160

Image not found

2-Benzylmalonate

Measured: 121

Predicted: 169

Image not found

Benzoic acid, 2-(
carboxymethoxy)-

Measured: 191

Predicted: 191

Image not found

Terephthalic acid

Measured: 313

Predicted: 268

Image not found

o-Phenylenediacetic acid

Measured: 151

Predicted: 177