

Docusate sodium
577-11-7 | DTXSID8022959

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: 162 °C

Global applicability domain: Inside

Local applicability domain index: 3.03e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

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Docusate sodium

Measured: 176

Predicted: 162

[Image not found](#)

O,O-Diethyl dithiophosphate

Measured: -10.0

Predicted: 1.00e-01

[Image not found](#)

Fumagillin

Measured: 195

Predicted: 182

[Image not found](#)

Trepibutone

Measured: 151

Predicted: 146

[Image not found](#)

Isofenphos

Measured: -12.0

Predicted: -0.602