

Docosate 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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 326 °C

Global applicability domain: Outside

Local applicability domain index: 1.45e-01

Confidence level: 5.48e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 2-benzoyl-

Measured: 261

Predicted: 309

Image not found

Benzoic acid, 2-phenoxy-

Measured: 355

Predicted: 325

Image not found

Linoleic acid

Measured: 365

Predicted: 361

Image not found

Eicosanoic acid

Measured: 328

Predicted: 332

Image not found

2,4-DB

Measured: 324

Predicted: 306