

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.11e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.12e-01

Confidence level: 3.15e-01

Nearest Neighbors from the Training Set

Image not found

Hexaconazole

Measured: 4.13e-09

Predicted: 3.12e-07

Image not found

2,4,6-Trichlorobiphenyl

Measured: 6.30e-04

Predicted: 7.09e-04

Image not found

Diflubenzuron

Measured: 3.67e-08

Predicted: 3.96e-10

Image not found

Bentazone

Measured: 3.00e-06

Predicted: 4.80e-07

Image not found

1,6-Dibromodibenzo-p-dioxin

Measured: 1.62e-05

Predicted: 1.57e-06