

Dantrolene
7261-97-4 | DTXSID7022881

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: 268 °C

Global applicability domain: Inside

Local applicability domain index: 3.34e-01

Confidence level: 4.72e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dantrolene

Measured: 280

Predicted: 268

[Image not found](#)

Nitrofurantoin

Measured: 263

Predicted: 253

[Image not found](#)

Oryzalin

Measured: 141

Predicted: 155

[Image not found](#)

Niridazole

Measured: 261

Predicted: 244

[Image not found](#)

Enprofylline

Measured: 288

Predicted: 263