

PUBCHEM_54605649

40730-78-7 | DTXSID90714109

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: 187 °C

Global applicability domain: Inside

Local applicability domain index: 3.78e-01

Confidence level: 6.04e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Sulfameter

Measured: 215

Predicted: 194

[Image not found](#)

Sulfamethoxypyridazine

Measured: 183

Predicted: 189

[Image not found](#)

Sulfachloropyridazine

Measured: 187

Predicted: 199

[Image not found](#)

Sulfadimethoxine

Measured: 204

Predicted: 196