

PUBCHEM_54609806

3698-87-1 | DTXSID60715027

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.18

Global applicability domain: Outside

Local applicability domain index: 1.02e-01

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

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4-Hydroxybenzoic acid

Measured: 8.08

Predicted: 7.78

[Image not found](#)

Salicylic acid

Measured: 7.44

Predicted: 7.60

[Image not found](#)

Phenacetin

Measured: 9.59

Predicted: 9.23

[Image not found](#)

Diphenylamine

Measured: 7.64

Predicted: 8.73

[Image not found](#)

Methylparaben

Measured: 8.57

Predicted: 7.06