

Bromacil
314-40-9 | DTXSID4022020

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: 6.71e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.98e-01

Confidence level: 4.91e-01

Nearest Neighbors from the Training Set

Image not found

Perfluorotributylamine

Measured: 3.07e-07

Predicted: 1.12

Image not found

Chloropropylate

Measured: 4.70e-07

Predicted: 3.62e-07

Image not found

3-Methyladenine

Measured: 1.10e-05

Predicted: 9.30e-10

Image not found

2-Hydroxyanthraquinone

Measured: 7.11e-04

Predicted: 4.19e-10

Image not found

Barban

Measured: 3.75e-05

Predicted: 1.55e-06