

Ethylparaben
120-47-8 | DTXSID9022528

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: 5.34e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.70e-01

Confidence level: 3.70e-01

Nearest Neighbors from the Training Set

Image not found

Isopentyl benzoate

Measured: 5.90e-06

Predicted: 4.01e-02

Image not found

Pyrethrin II

Measured: 1.04e-05

Predicted: 3.95e-07

Image not found

Butyl phenyl ether

Measured: 1.08e-03

Predicted: 5.92e-01

Image not found

MCPA

Measured: 8.25e-05

Predicted: 1.19e-06