

butyl 1-naphthoate
3007-95-2 | DTXSID10289046

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: 3.28e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.17e-01

Confidence level: 6.68e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl cinnamate

Measured: 1.00e-05

Predicted: 1.73e-02

Image not found

Clorophene

Measured: 2.24e-04

Predicted: 1.28e-05

Image not found

Butam

Measured: 1.19e-06

Predicted: 8.05e-04

Image not found

Heptenophos

Measured: 1.72e-04

Predicted: 3.05e-04

Image not found

Nonylphenyl diphenyl
phosphate, mixed isomers

Measured: 1.72e-04

Predicted: 8.08e-09