

(e)-1-(4-ethylphenyl)-2-phenyldiazene
61653-37-0 | DTXSID20295936

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: 1.74e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 5.22e-01

Nearest Neighbors from the Training Set

Image not found

Pentylcyclohexane

Measured: 2.00e-06

Predicted: 6.06e-01

Image not found

Bibenzyl

Measured: 3.61e-04

Predicted: 7.42e-03

Image not found

4-Aminoazobenzene

Measured: 7.00e-08

Predicted: 1.49e-06

Image not found

p-Ethylacetophenone

Measured: 3.92e-04

Predicted: 3.30e-01

Image not found

1,1':4',1"-Terphenyl

Measured: 6.11e-04

Predicted: 7.62e-06