

Ethanone, 1-(3-hydroxyphenyl)-
121-71-1 | DTXSID5059533

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: 3.79e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.91e-01

Confidence level: 3.97e-01

Nearest Neighbors from the Training Set

Image not found

2-Ethylhexanal

Measured: 1.13e-04

Predicted: 2.64

Image not found

2-Methylcyclohexanone

Measured: 9.95e-06

Predicted: 1.70

Image not found

2-Methylbenzoic acid

Measured: 6.60e-04

Predicted: 8.09e-04

Image not found

2-Ethylphenol

Measured: 5.93e-01

Predicted: 6.07e-02