

Methyl-d1 radical, oxo-
24286-05-3 | DTXSID90179017

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: 817 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.84e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

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1,2-Propadiene

Measured: 10400

Predicted: 1730

Image not found

Acetonitrile

Measured: 902

Predicted: 61.0

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3,3-dichloro-1,1,1,2,2-pentafluoropropane

Measured: 63.4

Predicted: 483

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Propane, 2-iodo-

Measured: 1610

Predicted: 35.2

Image not found

Arecoline

Measured: 232

Predicted: 1.33e-01