

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.49e-01

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 6.82e-01

Nearest Neighbors from the Training Set

Image not found

Formaldehyde

Measured: 0.35

Predicted: 2.38e-01

Image not found

Methyl formate

Measured: 0.03

Predicted: -0.0580

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HFC-41

Measured: 0.51

Predicted: 3.18e-01

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Methanol

Measured: -0.770

Predicted: -0.606

Image not found

Ethylene oxide

Measured: -0.300

Predicted: -0.259