

Aldicarb
116-06-3 | DTXSID0039223

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 38.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 6.30e-01

Nearest Neighbors from the Training Set

Image not found

Aldicarb

Measured: 31.6

Predicted: 38.0

Image not found

Ethyl phenylacetate

Measured: 77.6

Predicted: 103

Image not found

2-Phenylethyl acetate

Measured: 77.6

Predicted: 98.8

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Aldicarb sulfoxide

Measured: 3.63

Predicted: 8.06

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Ethyl 4-methylbenzoate

Measured: 389

Predicted: 150