

Phosphonothioic acid, methyl-, O,o-diethyl ester
6996-81-2 | DTXSID10220237

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 153 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.32e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

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Acetamide, N-(4-bromophenyl)-

Measured: 89.1

Predicted: 93.9

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Acetamide, N-(3-bromophenyl)-
(9CI)

Measured: 102

Predicted: 77.2

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3,4-Dichloroacetanilide

Measured: 219

Predicted: 111

Image not found

Etridiazole

Measured: 1000

Predicted: 82.5

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bis(2-Chloro-1-methylethyl) ether

Measured: 46.8

Predicted: 53.2