

Phosphonic acid, vinyl-, diethyl ester
682-30-4 | DTXSID70218372

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.43e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.94e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

Image not found

2-Vinylpyridine

Measured: 5.67e-11

Predicted: 5.45e-11

Image not found

2-Methyl-3-buten-2-ol

Measured: 6.48e-11

Predicted: 5.95e-11

Image not found

Ethyl acrylate

Measured: 1.60e-11

Predicted: 1.75e-11

Image not found

Isoprene

Measured: 1.01e-10

Predicted: 9.49e-11