

Diisopropyl fluorophosphate
55-91-4 | DTXSID1040667

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 96.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.94e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

Image not found

(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3

Image not found

3-Bromophenylurea

Measured: 132

Predicted: 114

Image not found

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

Measured: 102

Predicted: 77.2

Image not found

Methyl N-(3-chlorophenyl)carbamate

Measured: 141

Predicted: 94.1

Image not found

N-(4-Bromophenyl)urea

Measured: 115

Predicted: 122