

1,1,1,3,3-Pentafluoro-3-(1,2,2,2-tetrafluoroethoxy)propan-2-one
88457-11-8 | DTXSID00748238

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 206 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.01e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

Image not found

Mipafox

Measured: 41.2

Predicted: 1.79e-03

Image not found

Fenfuram

Measured: 387

Predicted: 1.44e-06

Image not found

Mepronil

Measured: 664

Predicted: 3.04e-07

Image not found

Benzene, 1-fluoro-2-(trifluoromethyl)-

Measured: 213

Predicted: 23.4

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Thiobencarb

Measured: 193

Predicted: 1.60e-05