

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane
26103-08-2 | DTXSID60448843

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 1.86

Global applicability domain: Inside

Local applicability domain index: 4.42e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

Image not found

Isoflurane

Measured: 2.06

Predicted: 2.08

Image not found

Enflurane

Measured: 2.10

Predicted: 2.02

Image not found

1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 1.66

Predicted: 1.56

Image not found

Ethane, hexafluoro-

Measured: 2.00

Predicted: 1.91

Image not found

Hexafluoroacetone

Measured: 1.46

Predicted: 1.55