

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

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: 210 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found

m-Xylene

Measured: 178

Predicted: 246

Image not found

ortho-Xylene

Measured: 178

Predicted: 249

Image not found

Ethylbenzene

Measured: 170

Predicted: 271

Image not found

1,3,5-Trimethylbenzene

Measured: 661

Predicted: 493

Image not found

Toluene

Measured: 117

Predicted: 87.4