

Ethyl phenylacetate
101-97-3 | DTXSID6044353

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: 103 L/kg

Global applicability domain: Inside

Local applicability domain index: 8.24e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl phenylacetate

Measured: 77.6

Predicted: 103

[Image not found](#)

2-Phenylethyl acetate

Measured: 77.6

Predicted: 98.8

[Image not found](#)

Ethyl 4-methylbenzoate

Measured: 389

Predicted: 150

[Image not found](#)

Ethylparaben

Measured: 162

Predicted: 98.6

[Image not found](#)

Butanamide, N-phenyl-

Measured: 51.3

Predicted: 67.1