

D-Galacturonic acid
685-73-4 | DTXSID2042646

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 9.33e-12 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.28e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

Image not found

Dimethyl glutarate

Measured: 3.30e-12

Predicted: 3.76e-12

Image not found

Dimethyl succinate

Measured: 1.40e-12

Predicted: 1.93e-12

Image not found

(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11