

2-hydroxy-3-methyl-2-(propan-2-yl)butanoic acid
5438-17-5 | DTXSID50280375

Model Performance

Model	Data
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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: 1.12e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.55e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

Image not found

2-Ethoxyethyl isobutyrate

Measured: 1.35e-11

Predicted: 1.28e-11

Image not found

Ethyl 3-ethoxypropionate

Measured: 2.29e-11

Predicted: 1.63e-11

Image not found

Ethyl lactate

Measured: 3.90e-12

Predicted: 4.80e-12

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

Image not found

Butyl butyrate

Measured: 1.06e-11

Predicted: 1.06e-11