

Butanoic acid, propyl ester
105-66-8 | DTXSID6059318

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: 6.98e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.60e-01

Confidence level: 9.17e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic acid, propyl ester

Measured: 7.41e-12

Predicted: 6.98e-12

Image not found

Pentyl acetate

Measured: 7.55e-12

Predicted: 6.38e-12

Image not found

Butyl butyrate

Measured: 1.06e-11

Predicted: 1.06e-11

Image not found

Ethyl butyrate

Measured: 4.94e-12

Predicted: 4.78e-12

Image not found

Propyl propionate

Measured: 4.02e-12

Predicted: 4.74e-12