

Bromacil
314-40-9 | DTXSID4022020

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: 1.20e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.45e-01

Confidence level: 8.48e-01

Nearest Neighbors from the Training Set

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

Image not found

Dimethyl glutarate

Measured: 3.30e-12

Predicted: 3.76e-12

Image not found

2-Ethoxyethyl isobutyrate

Measured: 1.35e-11

Predicted: 1.28e-11