

3-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-1-ol
6318-30-5 | DTXSID40282782

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.10

Global applicability domain: Inside

Local applicability domain index: 4.70e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

[Image not found](#)

1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

[Image not found](#)

2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35

[Image not found](#)

1,3-Benzenedimethanamine

Measured: 2.69

Predicted: 4.58

[Image not found](#)

Bromacil

Measured: 3.24

Predicted: 2.87