

Benzene, 1,1'-(1,3-propanediylbis(oxy))bis-
726-44-3 | DTXSID20222924

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: 26.4

Global applicability domain: Inside

Local applicability domain index: 4.29e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isoamyl ether

Measured: 170

Predicted: 137

[Image not found](#)

N,N-Diethylaniline

Measured: 102

Predicted: 12.8

[Image not found](#)

Isoproc carb

Measured: 8.91

Predicted: 13.6

[Image not found](#)

Menthol

Measured: 10.8

Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5