

1,3-diphenyl-1,3-diazetidone
74949-76-1 | DTXSID60321268

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: 113

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

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2,2'-Dithiobisbenzothiazole

Measured: 26.3

Predicted: 24.5

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N,N-Diethylaniline

Measured: 102

Predicted: 12.8

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Isoamyl ether

Measured: 170

Predicted: 137

[Image not found](#)

2-
(Thiocyanomethylthio)benzothiazole

Measured: 209

Predicted: 13.0

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Disulfoton

Measured: 219

Predicted: 151