

10,11-Dihydro-5H-dibenz(b,f)azepin-5-amine
7458-07-3 | DTXSID00225559

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: 6.97

Global applicability domain: Inside

Local applicability domain index: 4.48e-01

Confidence level: 5.68e-01

Nearest Neighbors from the Training Set

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Molinate

Measured: 25.7

Predicted: 14.8

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4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69

[Image not found](#)

Isophorone

Measured: 2.00

Predicted: 3.19

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N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 52.5

Predicted: 17.5

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Triallylamine

Measured: 3.55

Predicted: 4.23