

Psicofuranine
1874-54-0 | DTXSID80172052

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.60

Global applicability domain: Inside

Local applicability domain index: 4.50e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

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2-(¹⁵N)Amino-9-[(2xi)-beta-D-threo-pentofuranosyl]
(2-¹³C,1-¹⁵N)-3,9-dihydro-6H-purin-6-one

Measured: -1.90

Predicted: -1.32

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Adenosine

Measured: -1.05

Predicted: -1.46

[Image not found](#)

Inosine

Measured: -2.10

Predicted: -1.51

[Image not found](#)

N-[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]-2-(2-nitroimidazol-1-yl)acetamide

Measured: -1.77

Predicted: -1.83