

Acibenzolar-S-methyl
135158-54-2 | DTXSID1032519

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 121 °C

Global applicability domain: Inside

Local applicability domain index: 4.43e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found

Acibenzolar-S-methyl

Measured: 133

Predicted: 121

Image not found

Clotiazepam

Measured: 119

Predicted: 91.1

Image not found

2-(Morpholin-4-ylidithio)-1,3-benzothiazole

Measured: 135

Predicted: 117

Image not found

Benzenesulfonamide, N,4-dimethyl-N-nitroso-

Measured: 60.0

Predicted: 60.3

Image not found

N-Oxydiethylenebenzothiazole-2-sulfenamide

Measured: 85.0

Predicted: 90.5