Principal Component Regression Report

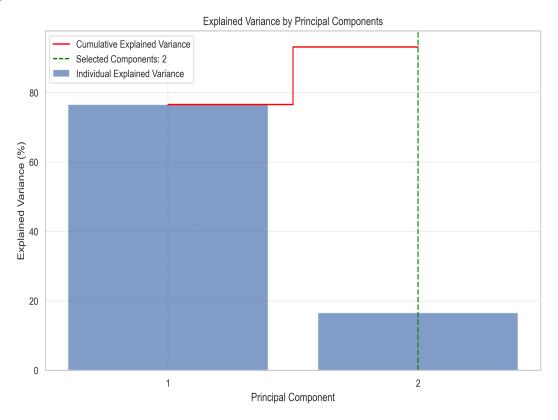
Dataset Information

Number of observations: 18 Number of variables: 73

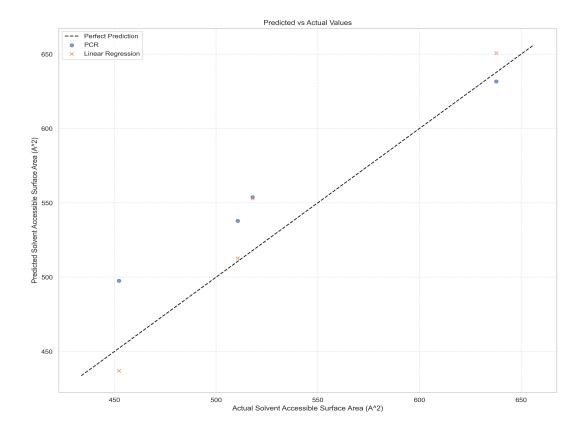
Target variable: Solvent Accessible Surface Area (A^2)

PCR Results

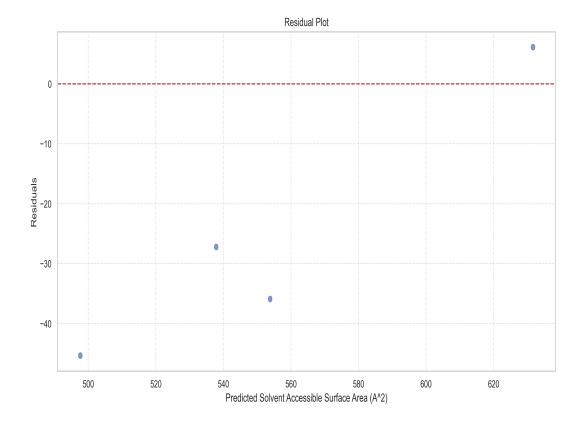
Explained Variance



Predicted vs Actual Values



Residuals Plot



Model Coefficients

Feature	PCR Coefficient	LR Coefficient
Molar mass	-0.2374	-1.6692
Atom count	0.0385	-3.8248
Heavy atom count	0.0058	0.4371
Rotatable bond count	0.0094	-0.2465
Ring count	0.0008	0.2261
Aromatic ring count	0.0007	1.3590
FSP3	0.0000	0.1251
Hydrogen bond acceptor count	0.0002	0.7409
Topological polar surface area	-0.0186	-0.7685
Polarizability	0.0168	1.2906
Molar refractivity	0.0396	-1.8489
HLB	0.0071	1.1960
logP	0.0003	2.1942
Van der Waals Volume (A^3)	0.1242	2.7548

Topological Polar Surface Area (A^2) Topological Polar Surface Area (A^2) Minimum Projection Area (A^2) Maximum Projection Area (A^2) Maximum Projection Area (A^2) Minimum projection radius (A) Monoce Minimum projection radius (A) LogP LogP Dounce Molecular Weight Dounce TPSA No. of Rotatable Bonds No Ratio No Ratio Number of Rings Number of Rings Number of Rings (size 6) Parachor Density Polarizability.1 Molar Volume Molar Volume No of Rotatable Bonds (1) Molar Refractivity No. of Rotatable Bonds No Ratio Dounce Dounce Dounce No Rotatable Rome Dounce Dounce	Van der Wasia Surface Area (AA2)	0.2052	2 9009
Minimum Projection Area (A^2) 0.0155 -3.1992 Maximum Projection Area (A^2) 0.0571 0.0620 Minimum projection radius (A) 0.0020 0.5102 Maximum projection radius (A) 0.0062 1.1009 LogD at pH 7.4 0.0003 2.2061 LogP 0.0034 2.3900 Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Refraction 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 </td <td>Van der Waals Surface Area (A^2)</td> <td>0.2952</td> <td>2.8008</td>	Van der Waals Surface Area (A^2)	0.2952	2.8008
Maximum Projection Area (A^2) 0.0571 0.0620 Minimum projection radius (A) 0.0020 0.5102 Maximum projection radius (A) 0.0062 1.1009 LogD at pH 7.4 0.0003 2.2061 LogP 0.0034 2.3900 Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0003 0.3317 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 <t< td=""><td>1 3</td><td></td><td></td></t<>	1 3		
Minimum projection radius (A) 0.0020 0.5102 Maximum projection radius (A) 0.0062 1.1009 LogD at pH 7.4 0.0003 2.2061 LogP 0.0034 2.3900 Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polar	. , ,		
Maximum projection radius (A) 0.0062 1.1009 LogD at pH 7.4 0.0003 2.2061 LogP 0.0034 2.3900 Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume	, ,		
LogD at pH 7.4 0.0003 2.2061 LogP 0.0034 2.3900 Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1)	. , , , , ,		
LogP	Maximum projection radius (A)		1.1009
Molecular Weight -0.2374 0.5399 No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680	LogD at pH 7.4	0.0003	2.2061
No. of Hydrogen Bond Acceptors -0.0012 0.9680 TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No.	LogP	0.0034	2.3900
TPSA 0.1883 -0.1737 No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatabl	Molecular Weight	-0.2374	0.5399
No. of Rotatable Bonds 0.0094 -0.2134 C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0007 -0.1623	No. of Hydrogen Bond Acceptors	-0.0012	0.9680
C Ratio 0.0007 -0.1623 N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Rat	TPSA	0.1883	-0.1737
N Ratio 0.0001 0.1409 NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0003 0.0231	No. of Rotatable Bonds	0.0094	-0.2134
NO Ratio -0.0003 0.0231 Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	C Ratio	0.0007	-0.1623
Hetero Ratio 0.0002 0.0811 Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	N Ratio	0.0001	0.1409
Halogen Ratio -0.0009 0.0802 Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	NO Ratio	-0.0003	0.0231
Number of Rings 0.0008 0.3317 Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Hetero Ratio	0.0002	0.0811
Number of Aromatic Rings 0.0006 0.6890 Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Halogen Ratio	-0.0009	0.0802
Number of Rings (size 6) 0.0005 1.0898 Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Number of Rings	0.0008	0.3317
Parachor 0.3024 0.3165 Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Number of Aromatic Rings	0.0006	0.6890
Index of Refraction 0.0001 -0.0229 Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Number of Rings (size 6)	0.0005	1.0898
Surface Tension 0.0025 -1.9566 Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Parachor	0.3024	0.3165
Density -0.0020 -0.0952 Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Index of Refraction	0.0001	-0.0229
Polarizability.1 0.0170 -0.4586 Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Surface Tension	0.0025	-1.9566
Molar Volume 0.1133 -2.5793 Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Density	-0.0020	-0.0952
Molar Refractivity 0.0428 -0.7802 Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Polarizability.1	0.0170	-0.4586
Molecular Weight (1) -0.2374 0.5399 No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Molar Volume	0.1133	-2.5793
No. of Hydrogen Bond Acceptors (1) -0.0012 0.9680 TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Molar Refractivity	0.0428	-0.7802
TPSA (1) 0.1883 -0.1737 No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	Molecular Weight (1)	-0.2374	0.5399
No. of Rotatable Bonds (1) 0.0094 -0.2134 C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	No. of Hydrogen Bond Acceptors (1)	-0.0012	0.9680
C Ratio (1) 0.0007 -0.1623 N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	TPSA (1)	0.1883	-0.1737
N Ratio (1) 0.0001 0.1409 NO Ratio (1) -0.0003 0.0231	No. of Rotatable Bonds (1)	0.0094	-0.2134
NO Ratio (1) -0.0003 0.0231	C Ratio (1)	0.0007	-0.1623
	N Ratio (1)	0.0001	0.1409
Hetero Ratio (1) 0.0002 0.0811	NO Ratio (1)	-0.0003	0.0231
	Hetero Ratio (1)	0.0002	0.0811

Halogen Ratio (1)	-0.0009	0.0802
Number of Rings (1)	0.0008	0.3317
Number of Aromatic Rings (1)	0.0006	0.6890
Number of Rings (size 6) (1)	0.0005	1.0898
Log(Koc)	0.0019	1.2887
Parachor (1)	0.3024	0.3165
Index of Refraction (1)	0.0001	-0.0229
Surface Tension (1)	0.0025	-1.9566
Density (1)	-0.0020	-0.0952
Polarizability (1)	0.0170	-0.4586
Molar Volume (1)	0.1133	-2.5793
Molar Refractivity (1)	0.0428	-0.7802
LogS (pH = 7,40)	-0.0035	0.7914
LogP (1)	0.0031	0.4870
LogD (pH = 7,40)	0.0031	0.4870
LogSw	-0.0035	0.7914
LogSw pH	0.0000	0.0000
LogP.1	0.0033	-0.0099
LogS (pH = 7,40) (1)	-0.0035	0.7914
LogD (pH = 7,40) (1)	0.0031	0.4870
LogS0	-0.0035	0.7914
LogP (2)	0.0031	0.4870