

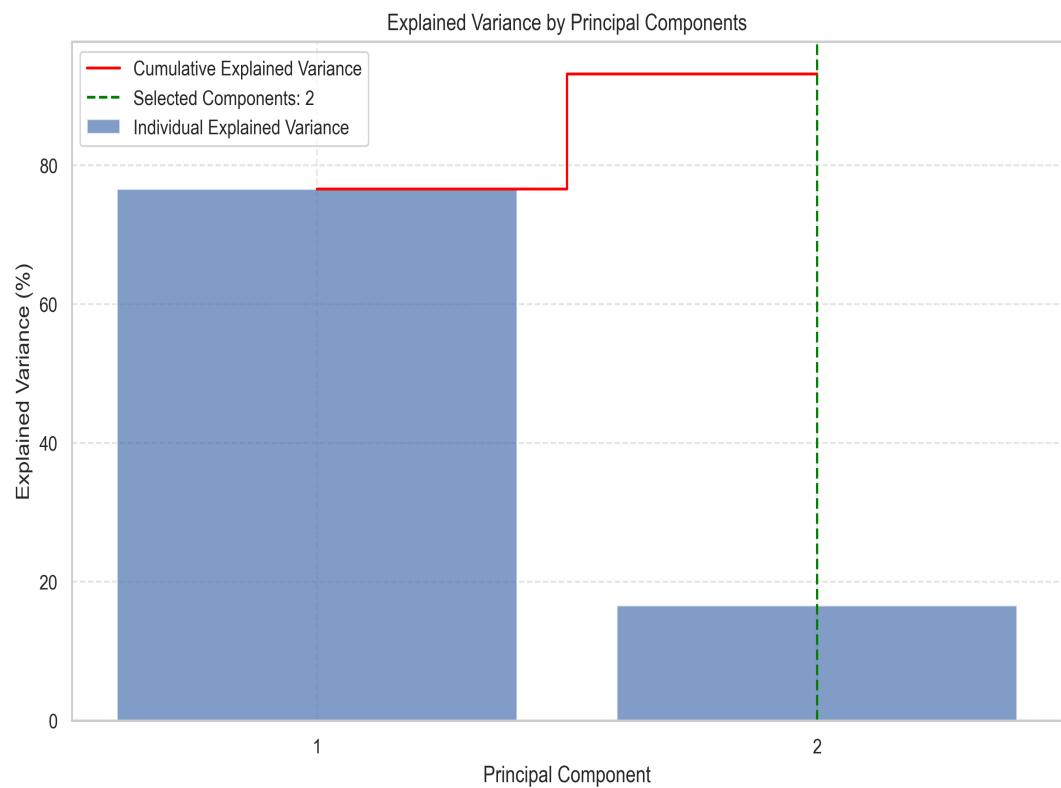
Principal Component Regression Report

Dataset Information

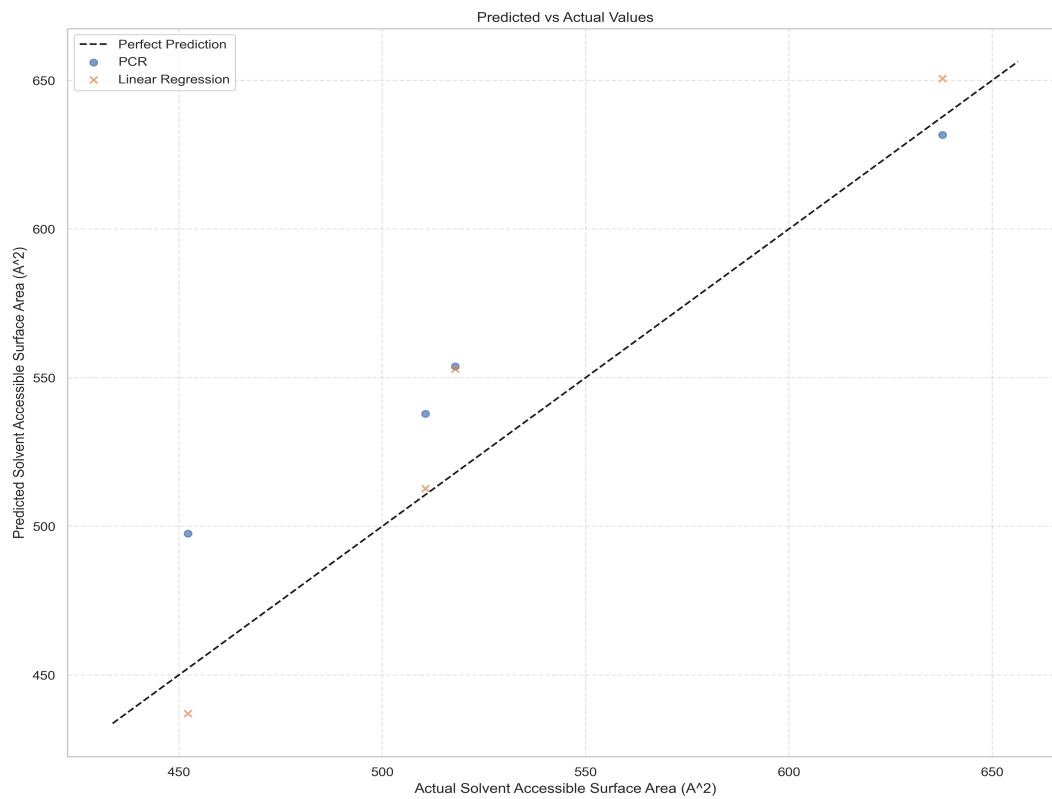
Number of observations: 18
Number of variables: 73
Target variable: Solvent Accessible Surface Area (A²)

PCR Results

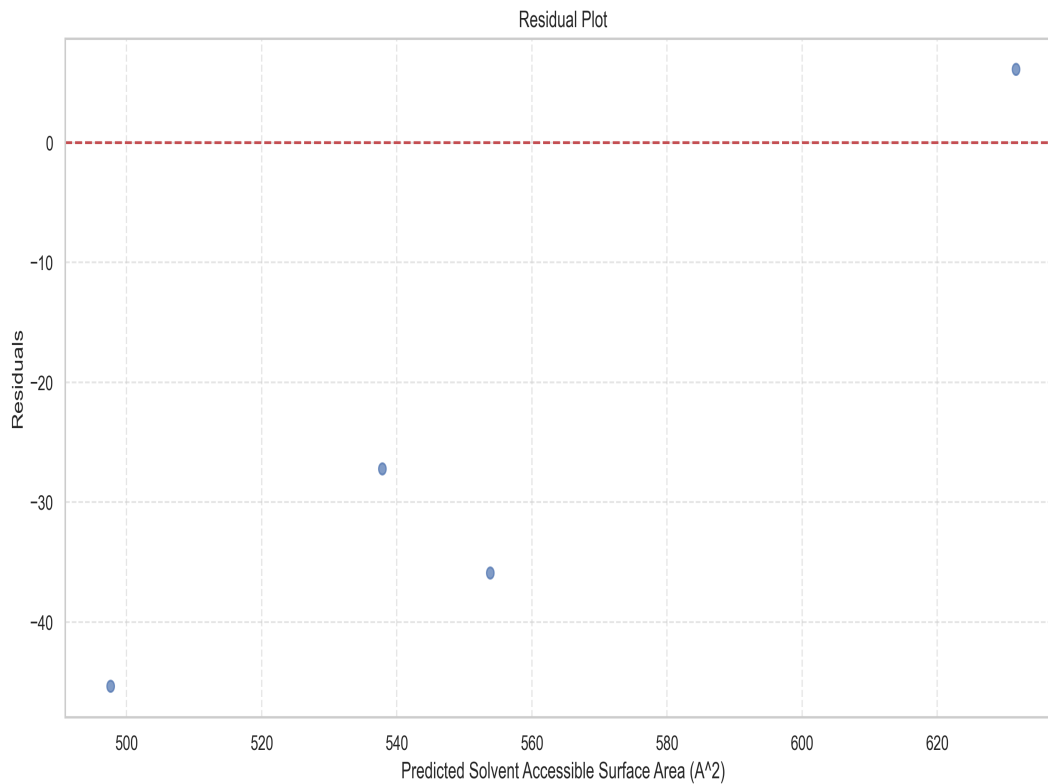
Explained Variance



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 (Å³)	0.1242	2.7548

Van der Waals Surface Area (A^2)	0.2952	2.8008
Topological Polar Surface Area (A^2)	-0.0186	-0.7653
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 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 (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