[66]: (67]: (67]: (77) [67]: (77)	oading the data df = pd.read_csv('https://raw.df MolLogP MolWt NumRotatableB 0 2.59540 167.850 1 2.37650 133.405 2 2.59380 167.850 3 2.02890 133.405 4 2.91890 187.375 139 1.98820 287.343 140 3.42130 286.114 141 3.60960 308.333 142 2.56214 354.815 143 2.02164 179.219 144 rows × 5 columns Pata preperation as X and Y y = df["logS"] y -2.180 -2.000 -1.740 -1.480 -3.040	onds AromaticF 0.0 0.0 1.0 1.0 1.0 2.0 4.0 3.0 1.0	
1: 1: 1: 1: 1: 1: 1: 1: 1: 1: 1: 1: 1: 1	1.144 1.140	onds AromaticF 0.0 0.0 1.0 1.0 1.0 2.0 4.0 3.0 1.0	0.000000 0.000000 0.000000 0.000000 0.000000
[73]: ; [73]: ; [73]: ; [73]: ; [73]: ; [74]: ; [74]: ; [74]: ; [74]: ;	MolLogP MolWt NumRotatableBo .07	inds AromaticPi 5.0 0.0 0.0 0.0 2.0 1.0 3.0 0.0 10.0 3.0	split(x,y,test_size=0.2,random_state=100) roportion 0.000000 0.000000 0.000000 0.000000 0.000000
1:	1.94040 145.161 1.123 1.98640 119.378 924 1.70062 108.140 1.14 1.76210 478.513 427 6.32820 276.338 711 0.04430 218.205 4 2.91890 187.375 948 3.56010 318.328 29 rows × 4 columns // Odel building inear Regression mporting the model from sklearn.linear_model impor fraining the model 1r = LinearRegression() 1r.fit(x_train,y_train) Applying the model to make y_lr_train_pred = lr.predict(x_ty_lr_train_pred) y_lr_train_pred = lr.predict(x_ty_lr_train_pred)	prediction	0.000000 0.750000 0.000000 1.000000 0.000000 0.000000 0.750000 0.750000
77]: a	-3.15082845, -4.33037208, -2.32734557, -4.19073421, -2.5501665, -3.26968347, -6.61955792, -2.99084623, -4.81736265, -0.86996608, -4.80953284, -4.17454084, -1.87131835, -2.45270806, -1.35216679, -0.16932277, -3.25501463, -5.31993586, -2.70343539, -3.70838271, -2.79842053, -1.38274662, -9.15826626, -6.52588866, -1.91317252, -2.81075595, -5.33227425, -3.88805074, -2.63405871, -1.80643013, -2.94105086, -3.02039211, -6.78423811, -2.34521849, -1.20887457, -3.4996968, -1.36030606, -1.97047357, -5.67559475, -3.04604495, -3.72245121, -5.49591484, -5.72200956, -0.20160041, -5.31993586, -5.30332414, -5.0001379, -1.29322696, -0.50844757, -2.79777831, -2.3552617, -4.47491213, -2.65582153, -2.03469435, -1.6454705, -1.67610138, -0.45142958, -3.70838271, -0.69767632, -4.61318325, -2.071356, -2.52212098, -3.0712261, -5.04235077, -0.14035732, -2.15201095, -3.87977779, -1.17409032, -6.52588866, -2.37600268, -1.08806317, -2.17972634, -4.38095601, -6.16274514, -2.41257831, -1.21383508, -0.07359075, -2.97947129, -6.51455759, -4.60929775, -4.91887429, -1.5001642, -3.58407147, -7.22253774, -8.54996931, -2.63926987, -1.76204643, -2.04984044, -4.91209304, -1.84841838, -1.6049836, -3.31107991, -4.63133161, -2.5020505, -1.96622986, -1.24556874, -1.73602998, -4.74777582, -3.52116416, -1.03137202, -2.45036038, -1.69652767, -5.04235077, -5.	-4.16684323 -1.43700682 -2.63904005 -2.78911367 -2.36975061 -7.09025955 -1.95444152 -3.07252433 -6.05237002 -0.4733928 -2.4987341 -4.3267103 -1.75832085 -1.14056747 0.70432882 -4.18615661 -2.01312164 -3.11841945 -4.98602607 -2.63177729 -5.17135083 -3.39797976 -0.54441899 -4.68554881 -4.9018288 -3.40409244 -1.37020598 -3.82343254 -2.25004084 -3.21804175 -2.53209123 -5.16155398 -4.57622144 -3.90580754 -5.38735798 -3.67042165 -1.37566371 -5.75210573 -2.77794109 -3.43909806 -3.36134518 -2.55131925 -0.40922333 -1.35467792 -6.42989154 -3.11841945 -4.69327814 -1.04661836 -2.04067926 -2.35789126 -2.35789126 -2.35789126 -2.35789126 -2.35789126 -2.35789126 -2.35789126 -2.7183962	0. 13858853, -1. 6269208 , -5. 04235877, -2. 29737089, -5. 04235877, -7. 39625955, -3. 58184724, -1. 373720553, -3. 58184724, -1. 373720553, -3. 58184724, -1. 373720553, -1. 6269203, -2. 4269203, -1. 6269203, -2. 4269203, -1. 6269203, -2. 4269203, -1. 6269203, -2. 4269203, -2. 1. 6269203, -3. 9595833, -3. 8376754, -3. 7975846, -3. 42556824, -4. 79186802, -5. 6246623, -4. 79186802, -3. 8376754, -3. 37778346, -3. 42556824, -4. 79186802, -3. 8256884, -3. 3928886, -2. 2299858, -3. 9928886, -2. 2299858, -3. 9928886, -2. 2299858, -3. 9928886, -2. 2299858, -3. 9928886, -2. 2298689, -3. 9928886, -2. 2298689, -3. 9928886, -2. 2898899, -3. 9928886, -2. 2898899, -3. 9928886, -2. 2898899, -3. 9928886, -2. 2898899, -3. 18778546, -3. 8387918, -3. 9928894, -3. 8387918, -3. 99389425, -3. 187782444, -3. 8387847, -4. 57827144, -3. 69389427, -4. 57827144, -3. 69389427, -4. 57827144, -3. 7938948, -1. 1987915, -3. 40889244, -1. 1917729, -2. 54472894, -1. 1917729, -2. 54472894, -1. 1917729, -2. 54472894, -1. 1917729, -2. 98487788, -1. 18269384, -3. 7918943, -2. 13889439, -3. 7918943, -2. 13889439, -3. 7918943, -2. 13889439, -3. 4089244, -3. 8891039, -3. 4089244, -3. 8891039, -3. 4089244, -3. 8891039, -3. 4089245, -3. 19389944, -3. 37918943, -2. 1388943, -3. 40899345, -2. 11738284, -3. 40899345, -2. 11738284, -3. 40899345, -2. 11738284, -3. 40899345, -3. 118989926, -4. 78989926, -1. 18267762, -4. 79989784, -3. 484495, -1. 192483329, -3. 4899242, -4. 18938339, -3. 8899240, -4. 18938339, -3. 8899240, -4. 18938339, -3. 8899240, -4. 18938339, -3. 8899240, -4. 18938339, -3. 8899240, -4. 18938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4. 19938339, -3. 8899240, -4
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[79]: \(\frac{1}{3} \)	-5.76437127e+00, -4.16422 -1.12679105e-02, -2.34523 8.55886378e-01, -3.17679 -7.77785827e+00, -1.21764 -2.43898748e+00, -2.84034 -1.63103729e+00, -1.53182 -1.88300518e+00, -3.21582 -4.82308940e+00, -7.69116 -1.95444152e+00, -3.50194 -2.08189806e+00, -2.31652 -6.01555673e+00, -2.88308 -3.54726250e+00, -1.21055 -1.63103729e+00, -2.51604 -3.20864450e+00, -1.51412 -3.26968347e+00, -3.94492 -5.98734972e+00, -1.43716 -1.14179382e+00, -3.07736 -1.68737438e+00, -2.20396 -2.79173430e+00, -2.41564 -9.20407401e-02, -6.14209 -1.79874130e+00, -2.50544 -2.57788713e+00, -2.6375 -6.68946164e+00, -1.91112 -1.90219551e+00, -2.81396 -1.60816482e+00, -3.68123 1.13185484e+00, -1.69279 -2.99712058e+00, -5.79606 -5.29389899e-01, -3.53652 -4.47466933e+00, -3.63836 -5.30676136e+00, -2.39225 -3.11841945e+00, -2.39225 -3.11841945e+00, -2.39225 -3.18768831e+00, -3.77197 -2.59432621e+00, -5.38486 -1.87252408e+00, -2.25124 -6.06861986e+00, -1.89916 -2.79393037e+00, -4.76010 -2.86880150e+00, -2.70674 -3.85805633e+00, -3.63698 -4.78343575e+00, -1.48988 -4.36873484e+00, -1.89724 -1.73602998e+00, -2.34522 -1.87770440e+00, -3.70838	2068e+00, -3. 849e+00, -1. 292e+00, -5. 693e+00, -9. 2045e+00, -3. 220e+00, -3. 220e+00, -3. 2343e-01, -7. 244e+00, -7. 2480e+00, -4. 291e+00, -4. 291e+00, -4. 291e+00, -1. 313e+00, -4. 218e+00, -1. 218e+00, -3. 2035e+00, -3. 2045e+00, -4. 2075e+00, -4. 2075e+00, -4. 2075e+00, -3. 2045e+00, -4. 2075e+00, -1.	97.55516.74-09. 7. 8343/346-0-18. 9. 43890462-0-19. 1.4834212-
3. 88 5. 3. 7. 7. N. 80]:	7.020 79 -4.800 792 -3.240 Pame: logS, Length: 915, dtype: y_lr_train_pred Parray([-2.83668969, 0.84208401, -2.86103037, -2.32208333, -3.15082845, -4.33037208, -2.32734557, -4.19073421, -2.5501665, -3.26968347, -6.61955792, -2.99084623, -4.81736265, -0.86996608, -4.80953284, -4.17454084, -1.87131835, -2.45270806, -1.35216679, -0.16932277, -3.25501463, -5.31993586, -2.70343539, -3.70838271, -2.79842053, -1.38274662, -9.15826626, -6.52588866, -1.91317252, -2.81075595, -5.33227425, -3.88805074, -2.63405871, -1.80643013, -2.94105086, -3.02039211, -6.78423811, -2.34521849, -1.20887457, -3.4996968, -1.36030606, -1.97047357, -5.67559475, -3.04604495, -3.72245121, -5.49591484, -5.72200956, -0.20160041, -5.31993586, -5.30332414, -5.0001379, -1.29322696, -0.50844757, -2.79777831, -2.3552617, -4.47491213, -2.65582153, -2.03469435,	-0.50930302 -4.16684323 -1.43700682 -2.63904005 -2.78911367 -2.36975061 -7.09025955 -1.95444152 -3.07252433 -6.05237002 -0.4733928 -2.4987341 -4.3267103 -1.75832085 -1.14056747 0.70432882 -4.18615661 -2.01312164 -3.11841945 -4.98602607 -2.63177729 -5.17135083 -3.39797976 -0.54441899 -4.68554881 -4.9018288 -3.40409244 -1.37020598 -3.82343254	, -0.13058053, -1.6269208, , 5.0425877, -2.29737099, , 5.0425877, -2.29737099, , -2.59960064, -7.69925955,
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	-3.47393942, -1.35730748, -2.33668279, -3.15515412, -4.27331505, -0.41608127, -1.35467792, -5.35250249, -1.21120552, -1.41272408, -4.70222762, -4.20128488, -2.75272546, -6.40483191, -2.3552617, -1.97390964, 2.54283347, -2.57935977, -2.84523685, -5.79050585, -1.89701519, -3.04694269, -6.11716924, -7.16934656, -6.40483191, -2.05580278, -3.27180065, -2.72328327, -1.10853776, -1.49259585, -1.80643013, -8.46728525, -1.94336083, -1.87633593, -0.5325366, -7.5914365, -4.36890615, -1.91112045, -3.82343254, -3.84290966, -3.95353483, -2.51949142, -2.08049675, -1.57187693, -3.87977779, -1.08911411, -3.56321848, -6.67044148, -2.14897281, -4.05818764, -3.08706826, -4.24521459, -2.03122625, -3.11841945, -4.23480474, -2.75684478, -3.59418929, -5.68837433, -1.41666505, -1.9765392, -2.65599022, -2.46014399, -3.81993282, -3.25038467, -2.29452458, -3.70387135, -1.91317252, -2.137733, -3.81016932, -2.44235234, -2.90610261, -7.77785827, -2.55678026, -2.59432621, -3.79386016, -6.40483191, -2.42494059, -6.04136471, -2.12601292, -4.28342693, -1.08911411, -4.24790282, -3.86772233, -1.2281273, -3.40980857, -2.6111225, -2.35283034, -0.7271857, -1.62166167, -3.90123327, -1	-2.35283034 -0.81254078 -0.92992939 -4.61318325 -0.62894611 -3.75287911 -3.43858076 -3.31913336 -1.5372532 -0.72972899 -1.10327863 -1.96622986 -3.67078501 -2.53353851 -1.15572753 -4.32045753 -9.15826626 -2.15587374 -5.28950294 -1.75395277 -4.16972153 -3.79234971 -2.73044354 -1.51156575 -2.37140338 -6.52588866 -5.04235077 -2.14339849 -5.02111613 -2.67587664 -3.93774254 -5.64350181 -6.42099768 -1.31128145 -2.76845189 -2.74034339 -6.06602826 -1.32841939 -1.63103729 -2.6178098 -4.63837202 -3.7672691 -1.41272408 -4.19010154 -2.78518496	. 3. 0572287 . 2. 08226573, 2. 32158664 . 7. 23311902, 2. 38152139 . 2. 3845254, 3. 36770115 . 4. 54753068, 5. 46726289 . 2. 80323664, 2. 89485114 . 9. 44470271, 4. 35654614 . 7. 3998571, 0. 99788515 . 1. 49117202, 1. 49699589 . 5. 50256395, 4. 50417895 . 3. 41743224, 1. 48989892 . 2. 81722646, 3. 315163216 . 3. 6117265, 5. 54551991 . 2. 93180057, 1. 11363181 . 2. 90610261, 4. 7604141 . 1924372, 1. 11916129 . 2. 25604844, 3. 93576 . 2. 288737344, 4. 28 2944893 . 1. 97756736, 4. 1. 908960216 . 1. 76845244, 3. 394574 . 3. 41747271 . 3. 41747271 . 3. 18986021 . 1. 76845244, 4. 3. 9494893 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 97756736, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 1. 9776942, 4. 94989349 . 3. 51206653, 9. 24989349 . 1. 7672119, 9. 94989349 . 3. 51206613, 9. 1. 9788625, 9. 1. 4319936 . 3. 51206653, 9. 1. 94989349 . 3. 51206653, 9. 1. 94989349 . 3. 51206613, 9. 1. 94889349 . 1. 9777842, 9. 1. 958869376, 9. 1. 94889349 . 1. 9777842, 9. 1. 94889349 . 1. 9777842, 9. 1. 94889349 . 1. 9778942, 9. 1. 94889349 . 1. 9778942, 9. 1. 94889349 . 1. 9778942, 9. 1. 94889349 . 1. 948893763, 9. 1. 94889349 . 1. 948893763, 9. 1. 94889349 . 1. 94889376, 9. 1. 94889349 . 1. 94889376, 9. 1. 94889349 . 1. 94889376, 9. 1. 94889389 . 1. 94889376, 9. 1. 94889389 . 1. 94889376, 9. 1. 94889389 . 1. 94889376, 9. 1. 94889389 . 1. 94889376, 9. 1. 94889389 . 1. 94889376, 9. 1. 94889389 . 1. 94889378, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1. 94889389 . 1. 94889389, 9. 1
[81]: 1	-2.54406861, -1.91317252, -1.51148185, -1.14665655, -2.11738204, -3.42356884, -1.62653948, -4.00428682, -1.69531648, -5.54561991, -0.73579117, -1.90396018, -0.88717007, -4.50417895, -2.73044354, -1.62464083, -4.36658559, -2.68703435, -3.80377549, -2.93847429, -0.77056362, -2.37730267, -3.17308636, -4.36923501, -1.80406335, -1.80643013, -3.22132977, -6.70156561, -3.98606913, -1.89546347, // Odel perfomance from sklearn.metrics import means and the second sec	-1.77769503 -2.00855418 -2.49648251 -2.04784256 -7.77785827 -3.66566374 -3.93774254 -3.36099002 -5.54667039 -3.69840797 1.68379176 -0.44844001 -1.90447849 -5.44962012 -6.08789325	, -0. 79489376, -4.23915498, , -7.03862139, -2.74305517, , -2.1372074, -1.88151626, , -4.47943132, -2.61216962, , -2.13315833, -6.08238994, , -3.26337102, -3.5528319, , -2.31911758, -1.79407614, , -1.68087565, -4.17747099, , -2.4662831, -5.07481336, , -3.63698515, -2.77930842, , -3.2158222, -3.70838271, , -5.24894879, -6.52225128, , -5.52193556, -2.07398557, , -1.2561011, -3.35223802, , -3.88711135, -3.78407726]) On
[83]:	R R2 (train): 0.76450517746633 R MSE (test): 1.02069536608616 R R2 (test): 0.789161618856328 lr_results = pd.DataFrame(['Lir lr_results.columns = ["method", lr_results method training mse training	ear regression training mse ear regression mse egressor ch=2, random egressor ch=2, rand	gressor dom_state=100) state=100)
100 1 1 1 1 1 1 1 1 1	rf_results.columns = ["method", rf_results method training mse training r Random forest 1.028228 0.75966	n_squared_error(y_train, yyrf_train, yyrf_train, yrf_train, yrf_train, yrf_test, yrf_test_pred dom forest', "training msed 2 test mse to the square test for the squ	y_rf_train_pred) pred) f_test_pred) d) rf_train_mse,rf_train_r2,rf_test_mse,rf_test_r2]).transpose() e","training r2","test mse","test r2"] mest r2 09223
1 (108)	Linear regression 1.007536 0.764 Random forest 1.028228 0.759 #df_models.reset_index(drop=True) Data visulaisation of the propert matplot library and Note import matplotlib.pyplot as plt import numpy as np #To draw plt.figure(figsize=(5,5)) # size	f prediction f	ne ph/***TCAE00" ,alpha=0.3) # "C=#7CAE00" represents the Green colour