| ID | name | RMSE | MAE | ME | $R^2$ | m | $\tau$ | ES |
|---|---|---|---|---|---|---|---|---|
| hmz0n | cosmotherm_FINE19 | 0.38 [0.48, 0.32] | 0.31 [0.40, 0.30] | -0.17 [0.01, -0.20] | 0.77 [0.90, 0.64] | 0.94 [1.08, 0.85] | 0.64 [0.88, 0.54] | 1.15 [1.28, 1.04] |
| gmoq5 | Global XGBoost-Based QSPR LogP Predictor | 0.39 [0.49, 0.35] | 0.34 [0.47, 0.30] | 0.01 [0.20, -0.02] | 0.74 [0.83, 0.65] | 0.99 [1.18, 0.88] | 0.59 [0.73, 0.49] | 0.69 [1.07, 0.34] |
| 3vqbi | cosmoquick_TZVP18+ML | 0.41 [0.59, 0.35] | 0.36 [0.53, 0.31] | -0.08 [0.25, -0.14] | 0.66 [0.93, 0.50] | 0.78 [0.82, 0.65] | 0.56 [0.92, 0.53] | 1.06 [1.20, 1.07] |
| sq07q | Local XGBoost-Based QSPR LogP Predictor | 0.47 [0.56, 0.39] | 0.41 [0.51, 0.34] | 0.03 [0.34, -0.10] | 0.64 [0.85, 0.63] | 0.92 [1.17, 0.90] | 0.56 [0.84, 0.60] | 0.60 [0.79, 0.46] |
| j8nwc | EC_RISM_wet_P1w+2o | 0.47 [0.75, 0.46] | 0.31 [0.56, 0.29] | 0.07 [0.28, 0.08] | 0.74 [0.96, 0.67] | 1.14 [1.38, 1.11] | 0.81 [1.00, 0.72] | 1.31 [1.45, 1.19] |
| dqxk4 | LogP_SMD_Solvation_DFT | 0.49 [0.56, 0.45] | 0.42 [0.50, 0.38] | 0.30 [0.41, 0.23] | 0.69 [0.86, 0.61] | 0.83 [1.27, 0.84] | 0.67 [0.76, 0.56] | 1.13 [1.21, 1.03] |
| hdpuj | RayLogP-II, a cheminformatic QSPR model predic... | 0.49 [0.58, 0.46] | 0.44 [0.56, 0.45] | -0.29 [-0.09, -0.39] | 0.74 [0.96, 0.73] | 1.02 [1.16, 1.00] | 0.67 [1.00, 0.65] | 0.91 [1.06, 0.88] |
| xxh4i | SM12-Solvation-Trained | 0.49 [0.64, 0.47] | 0.43 [0.59, 0.41] | 0.18 [0.36, -0.00] | 0.54 [0.81, 0.43] | 0.60 [0.81, 0.48] | 0.51 [0.73, 0.41] | 1.41 [1.47, 1.40] |
| ypmr0 | SM8-Solvation | 0.50 [0.63, 0.48] | 0.44 [0.60, 0.43] | 0.07 [0.30, -0.02] | 0.61 [0.81, 0.41] | 0.93 [1.23, 0.76] | 0.64 [0.85, 0.50] | 1.48 [1.49, 1.47] |
| vzgyt | rfs-logp | 0.50 [0.67, 0.47] | 0.38 [0.57, 0.35] | -0.35 [-0.22, -0.44] | 0.72 [0.85, 0.61] | 0.76 [0.93, 0.72] | 0.64 [0.80, 0.42] | 1.17 [1.34, 0.91] |
| yd6ub | S+logP | 0.51 [0.70, 0.52] | 0.41 [0.66, 0.40] | 0.09 [0.38, 0.11] | 0.63 [0.92, 0.51] | 0.99 [1.37, 1.02] | 0.53 [0.76, 0.35] | 0.73 [0.93, 0.59] |
| 7egyc | SMD-Solvation-Trained | 0.52 [0.58, 0.49] | 0.44 [0.50, 0.41] | 0.27 [0.41, 0.13] | 0.57 [0.63, 0.48] | 0.50 [0.59, 0.36] | 0.45 [0.72, 0.25] | 1.45 [1.47, 1.44] |
| 0a7a8 | ML Prediction using MD Feature Vector Trained ... | 0.53 [0.69, 0.46] | 0.43 [0.62, 0.31] | 0.32 [0.62, 0.24] | 0.62 [0.77, 0.35] | 0.74 [1.04, 0.51] | 0.45 [0.73, 0.22] | 1.01 [1.14, 0.84] |
| 7dhtp | LogP-prediction-method-name | 0.54 [0.66, 0.40] | 0.44 [0.60, 0.33] | 0.06 [0.17, -0.02] | 0.49 [0.87, 0.50] | 0.73 [1.04, 0.68] | 0.56 [0.79, 0.62] | 0.50 [0.81, 0.45] |
| qyzjx | EC_RISM_dry_P1w+2o | 0.54 [0.79, 0.42] | 0.46 [0.65, 0.40] | -0.15 [0.24, -0.25] | 0.73 [0.95, 0.60] | 1.22 [1.71, 1.18] | 0.78 [1.00, 0.76] | 1.22 [1.32, 1.16] |
| w6jta | ML Prediction using MD Feature Vector Trained ... | 0.56 [0.73, 0.43] | 0.46 [0.64, 0.35] | 0.32 [0.50, 0.17] | 0.53 [0.80, 0.47] | 0.62 [0.74, 0.57] | 0.51 [0.73, 0.31] | 1.12 [1.26, 1.05] |
| 5krdi | ZINC15 versus PM3 | 0.60 [0.65, 0.55] | 0.51 [0.57, 0.46] | -0.30 [-0.06, -0.35] | 0.63 [0.82, 0.59] | 1.03 [1.30, 0.93] | 0.60 [0.84, 0.55] | 0.37 [0.55, 0.21] |
| ji2zm | SM8-Solvation-Trained | 0.60 [0.70, 0.50] | 0.53 [0.64, 0.42] | 0.45 [0.59, 0.29] | 0.66 [0.91, 0.63] | 0.66 [0.98, 0.57] | 0.51 [0.84, 0.57] | 1.43 [1.44, 1.41] |
| gnxuu | ML Prediction using MD Feature Vector Trained ... | 0.61 [0.72, 0.58] | 0.51 [0.64, 0.43] | 0.40 [0.59, 0.28] | 0.53 [0.97, 0.47] | 0.57 [0.66, 0.55] | 0.51 [0.88, 0.37] | 1.10 [1.24, 1.04] |
| tc4xa | NHLBI-NN-5HL | 0.62 [0.78, 0.54] | 0.51 [0.73, 0.46] | 0.17 [0.54, 0.14] | 0.66 [0.92, 0.54] | 1.21 [1.52, 1.02] | 0.49 [0.88, 0.47] | 1.10 [1.35, 1.09] |
| 6cdyo | SM12-Solvation | 0.65 [0.86, 0.64] | 0.54 [0.81, 0.53] | -0.24 [-0.06, -0.41] | 0.52 [0.81, 0.52] | 0.93 [1.84, 0.82] | 0.53 [0.76, 0.42] | 0.78 [1.11, 0.67] |
| dbmg3 | GC-LSER | 0.70 [0.83, 0.61] | 0.60 [0.74, 0.54] | 0.42 [0.58, 0.30] | 0.47 [0.68, 0.25] | 0.75 [1.18, 0.31] | 0.38 [0.67, 0.22] | 1.43 [1.47, 1.41] |
| kxsp3 | PLS2 from NIST data and QM-generated QSAR Desc... | 0.74 [0.79, 0.60] | 0.62 [0.66, 0.48] | 0.48 [0.60, 0.39] | 0.36 [0.54, 0.07] | 0.54 [1.13, 0.15] | 0.35 [0.69, -0.02] | 0.71 [0.79, 0.54] |
| nh6c0 | Molecular-Dynamics-Expanded-Ensembles | 0.74 [0.81, 0.61] | 0.67 [0.74, 0.57] | 0.09 [0.26, -0.29] | 0.62 [0.89, 0.51] | 1.34 [1.66, 1.14] | 0.49 [0.68, 0.37] | 0.74 [0.94, 0.71] |
| kivfu | LogP-prediction-method-IEFPCM/MST | 0.78 [0.92, 0.58] | 0.56 [0.72, 0.40] | -0.03 [0.34, -0.17] | 0.41 [0.80, 0.42] | 0.97 [1.25, 0.95] | 0.45 [0.76, 0.35] | 1.07 [1.18, 1.02] |
| ujsgv | Alchemical-CGenFF | 0.82 [0.96, 0.70] | 0.67 [0.82, 0.55] | -0.31 [-0.03, -0.45] | 0.33 [0.80, 0.28] | 0.80 [1.48, 0.88] | 0.35 [0.80, 0.36] | 1.27 [1.36, 1.25] |
| wu52s | LogP-PLS-ECFC4_CSsep-Bayer | 0.83 [1.03, 0.77] | 0.72 [0.93, 0.67] | 0.70 [0.91, 0.65] | 0.55 [0.79, 0.49] | 0.54 [0.74, 0.51] | 0.56 [0.80, 0.42] | 0.42 [0.66, 0.31] |
| 5mahv | ML Prediction using MD Feature Vector Trained ... | 0.85 [1.04, 0.70] | 0.62 [0.88, 0.54] | -0.02 [0.31, -0.21] | 0.34 [0.58, 0.26] | 0.90 [0.98, 0.74] | 0.24 [0.58, -0.02] | 1.07 [1.12, 0.94] |
| g6dwz | NHLBI-NN-3HL | 0.85 [1.09, 0.90] | 0.72 [1.01, 0.76] | 0.35 [0.75, 0.26] | 0.52 [0.91, 0.17] | 1.18 [1.62, 0.77] | 0.45 [0.96, 0.22] | 0.84 [0.97, 0.69] |
| bqeuh | ISIDA-LSER | 0.87 [1.10, 0.72] | 0.66 [0.87, 0.54] | 0.25 [0.66, 0.04] | 0.01 [0.24, 0.02] | -0.05 [0.48, -0.09] | 0.02 [0.29, -0.15] | 1.33 [1.36, 1.28] |
| d7vth | UFZ-LSER | 0.87 [1.16, 0.75] | 0.78 [1.02, 0.67] | -0.65 [-0.32, -0.61] | 0.63 [0.75, 0.53] | 1.11 [1.30, 1.01] | 0.49 [0.72, 0.37] | 0.77 [1.04, 0.68] |
| 2mi5w | Alchemical-CGenFF | 0.95 [1.14, 0.91] | 0.81 [1.06, 0.81] | -0.30 [-0.02, -0.55] | 0.18 [0.34, 0.06] | 0.61 [0.87, 0.38] | 0.24 [0.40, -0.02] | 1.21 [1.32, 1.20] |
| qz8d5 | SMD-Solvation | 0.97 [1.14, 0.84] | 0.84 [1.05, 0.66] | 0.77 [1.05, 0.66] | 0.53 [0.84, 0.49] | 0.93 [1.48, 0.94] | 0.48 [0.86, 0.31] | 1.40 [1.45, 1.38] |
| kuddg | LogP-Pred-MTNN-GraphConv-Bayer | 0.97 [1.18, 0.86] | 0.89 [1.10, 0.79] | 0.89 [1.10, 0.79] | 0.67 [0.94, 0.46] | 0.71 [0.92, 0.66] | 0.53 [0.88, 0.36] | 0.17 [0.31, 0.17] |
| 2ggir | FS-AGM (Fast switching Annihilation/Growth Met... | 1.04 [1.23, 0.99] | 0.98 [1.16, 0.97] | -0.36 [0.08, -0.62] | 0.31 [0.90, 0.09] | 0.98 [1.74, 0.46] | 0.49 [0.92, 0.32] | 0.83 [0.93, 0.75] |
| y0xxd | FS-GM (Fast switching Growth Method) | 1.04 [1.50, 0.89] | 0.72 [1.22, 0.56] | 0.37 [0.93, 0.18] | 0.33 [0.95, 0.24] | 1.03 [1.96, 0.84] | 0.42 [0.91, 0.28] | 1.31 [1.42, 1.24] |
| dyxbt | B3PW91-TZ SMD set1 | 1.07 [1.31, 1.03] | 0.96 [1.19, 0.93] | 0.96 [1.19, 0.93] | 0.55 [0.88, 0.39] | 0.68 [1.05, 0.50] | 0.56 [0.88, 0.50] | -0.00 [0.01, -0.00] |
| mm0jf | LogP-prediction-SMD-HuangLab | 1.09 [1.17, 1.06] | 1.03 [1.16, 1.00] | 1.03 [1.16, 1.00] | 0.75 [0.96, 0.70] | 0.60 [0.80, 0.54] | 0.75 [0.96, 0.73] | 1.09 [1.18, 1.05] |
| h83sb | Linear Regression with B3LYP/6-31G+ | 1.12 [1.62, 1.10] | 0.87 [1.37, 0.89] | -0.21 [0.24, -0.49] | 0.00 [0.36, 0.01] | -0.02 [0.54, -0.38] | -0.16 [0.21, -0.42] | 0.33 [0.40, 0.13] |
| 3wvyh | Alchemical-CGenFF | 1.13 [1.68, 1.04] | 0.77 [1.16, 0.64] | 0.26 [0.97, 0.20] | 0.37 [0.44, 0.22] | 1.24 [1.82, 0.83] | 0.55 [0.69, 0.38] | 1.23 [1.38, 1.18] |
| f3dpg | PLS from NIST data and QM-generated QSAR Descr... | 1.17 [1.40, 0.95] | 0.92 [1.22, 0.67] | -0.85 [-0.41, -1.02] | 0.11 [0.33, 0.09] | 0.36 [0.75, 0.46] | 0.15 [0.52, 0.20] | 0.63 [1.06, 0.39] |
| zdj0j | Solvation-B3LYP | 1.21 [1.38, 1.22] | 1.13 [1.31, 1.13] | 1.13 [1.31, 1.13] | 0.64 [0.89, 0.63] | 0.86 [1.32, 0.69] | 0.64 [0.96, 0.48] | 0.08 [0.22, 0.09] |
| 25s67 | FS-AGM (Fast switching Annihilation/Growth Met... | 1.21 [1.43, 0.89] | 1.06 [1.19, 0.74] | -0.97 [-0.43, -1.03] | 0.63 [0.85, 0.31] | 1.33 [2.33, 0.81] | 0.45 [0.76, -0.25] | 0.79 [1.04, 0.59] |
| 7gg6s | MLR from NIST data and QM-generated QSAR Descr... | 1.27 [1.37, 1.16] | 1.00 [1.13, 0.82] | -1.00 [-0.69, -1.05] | 0.10 [0.38, 0.01] | 0.31 [0.45, 0.06] | 0.16 [0.44, -0.06] | 0.60 [1.04, 0.43] |
| pcv32 | Solvation- WB97X-D | 1.28 [1.50, 1.29] | 1.17 [1.45, 1.14] | 1.17 [1.45, 1.14] | 0.50 [0.80, 0.42] | 0.75 [1.10, 0.51] | 0.44 [0.80, 0.44] | 0.28 [0.54, 0.14] |
| hwf2k | Extended solvent-contact model approach | 1.28 [1.80, 1.14] | 0.93 [1.39, 0.82] | -0.09 [0.42, -0.33] | 0.12 [0.38, 0.02] | 0.68 [2.01, 0.10] | 0.31 [0.65, -0.13] | 0.48 [0.78, 0.35] |
| v2q0t | InterX_GAFF_WET_OCTANOL | 1.31 [1.52, 1.03] | 1.16 [1.40, 0.94] | -1.15 [-0.77, -1.18] | 0.70 [0.97, 0.59] | 1.31 [1.55, 1.25] | 0.64 [1.00, 0.56] | 1.34 [1.41, 1.31] |
| ggm6n | FS-GM (Fast switching Growth Method) | 1.32 [1.55, 1.15] | 1.16 [1.47, 1.03] | -1.15 [-0.97, -1.34] | 0.53 [0.76, 0.55] | 1.04 [1.35, 0.96] | 0.53 [0.74, 0.52] | 1.17 [1.37, 1.09] |
| rdsnw | EC_RISM_wet_P1w+1o | 1.32 [1.58, 1.17] | 1.15 [1.41, 1.01] | 1.15 [1.41, 1.01] | 0.78 [0.96, 0.71] | 1.51 [1.73, 1.44] | 0.75 [0.92, 0.76] | 0.98 [1.16, 0.89] |
| jjd0b | MD/S-MBIS-GAFF-TIP3P/MBAR/ | 1.35 [1.78, 1.35] | 1.13 [1.63, 1.14] | -1.09 [-0.75, -1.35] | 0.66 [0.92, 0.46] | 1.51 [1.92, 1.45] | 0.53 [0.96, 0.28] | 0.75 [1.02, 0.69] |
| 2tzb0 | EC_RISM_dry_P1w+1o | 1.38 [1.58, 1.17] | 1.21 [1.35, 1.10] | 1.21 [1.35, 1.10] | 0.79 [0.97, 0.57] | 1.58 [2.09, 1.55] | 0.75 [0.88, 0.73] | 1.00 [1.35, 0.93] |
| cr3hs | PLS3 from NIST data and QM-generated QSAR Desc... | 1.39 [2.01, 0.88] | 0.96 [1.49, 0.71] | 0.80 [1.34, 0.50] | 0.40 [0.67, 0.37] | 1.36 [2.54, 0.94] | 0.35 [0.83, 0.32] | 0.65 [0.84, 0.69] |
| ahmtf | B3PW91-TZ SMD kcl-wet-oct | 1.41 [1.68, 1.46] | 1.33 [1.63, 1.39] | 1.33 [1.63, 1.39] | 0.55 [0.84, 0.35] | 0.70 [1.23, 0.47] | 0.56 [1.00, 0.39] | -0.00 [-0.00, -0.00] |
| arw58 | DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.41 [1.86, 1.24] | 1.09 [1.57, 0.97] | 1.01 [1.57, 0.96] | 0.09 [0.38, 0.06] | -0.24 [-0.16, -0.34] | -0.20 [-0.15, -0.40] | -0.00 [-0.00, -0.00] |
| o7djk | B3PW91-TZ SMD wetoct | 1.42 [1.51, 1.37] | 1.34 [1.45, 1.27] | 1.34 [1.45, 1.27] | 0.55 [0.89, 0.45] | 0.70 [1.23, 0.55] | 0.56 [1.00, 0.36] | -0.00 [-0.00, -0.00] |
| fmf7r | dice | 1.44 [1.62, 1.22] | 1.25 [1.45, 1.07] | 0.26 [1.20, 0.06] | 0.05 [0.62, 0.02] | 0.47 [2.13, 0.03] | 0.10 [0.70, -0.12] | 0.32 [0.68, 0.20] |
| 4p2ph | DLPNO-Solv-ccCA | 1.44 [1.92, 0.98] | 1.12 [1.74, 0.70] | 1.04 [1.74, 0.69] | 0.09 [0.55, 0.03] | -0.26 [0.24, -0.44] | -0.26 [0.43, -0.52] | -0.00 [-0.00, -0.00] |
| 6fyg5 | Solvation-M062X | 1.50 [1.66, 1.45] | 1.44 [1.64, 1.37] | 1.44 [1.64, 1.37] | 0.69 [0.94, 0.65] | 0.93 [1.31, 0.79] | 0.71 [1.00, 0.58] | 0.05 [0.14, 0.02] |
| sqosi | MD-AMBER-dryoct | 1.69 [2.15, 1.52] | 1.42 [1.93, 1.22] | -1.40 [-1.13, -1.51] | 0.51 [0.74, 0.55] | 1.40 [2.28, 1.15] | 0.45 [0.80, 0.33] | 0.72 [0.93, 0.58] |
| rs4ns | BLYP/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.71 [1.66, 1.31] | 1.44 [1.41, 1.10] | 1.44 [1.41, 1.10] | 0.06 [0.14, 0.02] | -0.19 [0.16, -0.12] | -0.22 [0.30, -0.09] | 0.07 [0.27, -0.00] |
| c7t5j | PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.73 [2.06, 1.68] | 1.47 [1.87, 1.44] | 1.47 [1.87, 1.44] | 0.05 [0.32, 0.01] | -0.18 [0.10, -0.36] | -0.16 [0.26, -0.38] | -0.00 [-0.00, -0.00] |
| jc68f | PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.74 [2.32, 1.67] | 1.47 [2.03, 1.42] | 1.47 [2.03, 1.42] | 0.05 [0.61, 0.02] | -0.18 [-0.08, -0.32] | -0.16 [0.00, -0.28] | -0.00 [-0.00, -0.00] |
| 03cyy | Linear Regression-B3LYP/6-311G** | 1.75 [2.75, 0.84] | 1.11 [1.94, 0.61] | 0.03 [0.83, -0.58] | 0.00 [0.43, 0.01] | 0.12 [2.49, -0.22] | 0.09 [0.46, -0.13] | 0.36 [0.60, 0.27] |
| hsotx | B3LYP/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.81 [2.18, 1.50] | 1.56 [1.99, 1.26] | 1.56 [1.99, 1.26] | 0.07 [0.43, 0.01] | -0.19 [0.04, -0.28] | -0.20 [0.08, -0.27] | -0.00 [0.02, -0.00] |
| ke5gu | MD/S-MBIS-GAFF-SPCE/MBAR/ | 1.82 [2.31, 1.64] | 1.59 [2.14, 1.31] | -1.59 [-1.03, -1.67] | 0.62 [0.90, 0.61] | 1.54 [2.44, 1.60] | 0.53 [0.76, 0.48] | 0.49 [0.82, 0.49] |

| ID | name | RMSE | MAE | ME | R² | m | τ | ES |
|---|---|---|---|---|---|---|---|---|
| mwuua | MD-LigParGen-wetoct | 1.83 [2.09, 1.82] | 1.73 [2.06, 1.75] | -1.73 [-1.62, -1.87] | 0.41 [0.69, 0.41] | 0.67 [0.91, 0.59] | 0.48 [0.72, 0.38] | 0.49 [0.66, 0.46] |
| fe8ws | B3PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.83 [2.53, 1.86] | 1.58 [2.40, 1.61] | 1.58 [2.40, 1.61] | 0.06 [0.35, 0.11] | -0.18 [-0.12, -0.52] | -0.16 [0.31, -0.45] | -0.00 [-0.00, -0.00] |
| 5t0yn | PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.85 [2.07, 1.68] | 1.61 [1.78, 1.46] | 1.61 [1.78, 1.46] | 0.06 [0.56, 0.04] | -0.18 [0.12, -0.52] | -0.16 [0.14, -0.51] | -0.00 [-0.00, -0.00] |
| fyx45 | LogP-prediction-Drude-FEP-HuangLab | 1.85 [2.58, 1.41] | 1.25 [1.85, 1.09] | 0.65 [1.22, 0.43] | 0.63 [0.87, 0.50] | 2.63 [4.01, 1.99] | 0.67 [0.92, 0.62] | 0.80 [1.01, 0.78] |
| 6nmtt | MD-AMBER-wetoct | 1.87 [2.61, 1.58] | 1.65 [2.36, 1.49] | -1.65 [-1.23, -1.85] | 0.42 [0.79, 0.36] | 1.10 [1.74, 1.02] | 0.60 [0.92, 0.53] | 0.57 [0.86, 0.39] |
| eufcy | MD-LigParGen-dryoct | 1.99 [2.28, 1.88] | 1.88 [2.19, 1.75] | -1.77 [-1.39, -1.94] | 0.54 [0.73, 0.29] | 1.43 [3.10, 0.75] | 0.66 [0.88, 0.47] | 0.41 [0.57, 0.32] |
| tzzb5 | Alchemical-CGenFF | 2.12 [2.67, 1.93] | 1.87 [2.56, 1.67] | 1.43 [2.56, 0.94] | 0.20 [0.96, 0.09] | -0.76 [0.26, -1.15] | -0.20 [0.45, -0.63] | 0.66 [0.96, 0.65] |
| 3oqhx | MD-CHARMM-dryoct | 2.14 [2.48, 1.72] | 1.64 [2.19, 1.28] | 1.11 [2.10, 0.61] | 0.03 [0.14, 0.01] | -0.44 [0.78, -0.55] | 0.00 [0.40, -0.16] | 0.75 [0.99, 0.58] |
| bzeez | FS-AGM (Fast switching Annihilation/Growth Met... | 2.20 [2.53, 2.18] | 2.07 [2.49, 2.05] | -2.07 [-1.93, -2.36] | 0.63 [0.92, 0.54] | 1.39 [1.55, 1.30] | 0.53 [0.88, 0.38] | 0.23 [0.36, 0.10] |
| 5svjv | FS-GM (Fast switching Growth Method) | 2.26 [2.37, 1.99] | 2.14 [2.26, 1.89] | -2.03 [-1.58, -2.10] | 0.39 [0.90, 0.26] | 1.20 [1.69, 1.13] | 0.44 [0.98, 0.70] | 0.74 [0.90, 0.70] |
| ynquk | TWOVAR | 2.26 [2.48, 2.19] | 2.13 [2.47, 2.03] | 2.13 [2.47, 2.03] | 0.08 [0.83, 0.03] | 0.25 [0.63, 0.10] | 0.38 [0.92, 0.36] | 1.07 [1.19, 1.05] |
| padym | InterX_ARROW_2017_PIMD_WET_OCTANOL | 2.29 [2.47, 1.91] | 1.99 [2.28, 1.63] | 1.72 [2.02, 1.37] | 0.12 [0.57, 0.04] | -0.60 [0.52, -0.64] | -0.13 [0.19, -0.25] | 1.09 [1.21, 1.05] |
| pnc4j | LogP-prediction-Drude-Umbrella-HuangLab | 2.29 [2.65, 2.04] | 2.03 [2.56, 1.81] | 2.03 [2.56, 1.81] | 0.04 [0.32, 0.02] | 0.31 [0.76, 0.16] | 0.20 [0.45, 0.12] | 0.39 [0.63, 0.25] |
| odex0 | InterX_ARROW_2017_PIMD_SOLVENT2_WET_OCTANOL | 2.29 [2.89, 1.81] | 1.98 [2.82, 1.61] | 1.73 [2.57, 0.86] | 0.09 [0.42, 0.01] | -0.53 [0.23, -0.91] | -0.09 [0.57, -0.44] | 1.09 [1.30, 0.99] |
| fcspk | ARROW_2017_PIMD_SOLVENT2 | 2.40 [2.91, 2.15] | 2.10 [2.75, 1.79] | 1.97 [2.75, 1.66] | 0.11 [0.51, 0.04] | -0.50 [-0.23, -0.64] | -0.16 [0.10, -0.40] | 1.06 [1.15, 0.97] |
| 6cm6a | ARROW_2017_PIMD | 2.41 [2.70, 2.17] | 2.10 [2.49, 1.83] | 1.94 [2.32, 1.50] | 0.19 [0.41, 0.09] | -0.66 [-0.10, -0.64] | -0.27 [0.02, -0.59] | 1.06 [1.28, 1.04] |
| bq6fo | Extended solvent-contact model approach | 2.58 [2.86, 2.19] | 2.15 [2.47, 1.75] | 1.55 [1.95, 0.76] | 0.10 [0.36, 0.03] | 1.05 [2.06, 0.55] | 0.09 [0.54, -0.04] | 0.23 [0.31, 0.11] |
| 623c0 | MD-OPLSAA-wetoct | 2.67 [2.97, 2.37] | 2.53 [2.85, 2.32] | -2.53 [-2.20, -2.68] | 0.22 [0.67, 0.17] | 0.64 [0.92, 0.56] | 0.38 [0.63, 0.19] | 0.18 [0.24, 0.14] |
| 4nfzz | MD/S-HI-GAFF-TIP3P/MBAR/ | 2.67 [3.40, 2.66] | 2.44 [3.07, 2.40] | -2.44 [-2.24, -2.68] | 0.40 [0.53, 0.21] | 1.30 [1.60, 1.11] | 0.42 [0.58, 0.19] | 0.20 [0.32, 0.11] |
| eg52i | ARROW_2017 | 2.86 [3.75, 2.77] | 2.41 [3.61, 2.32] | 2.06 [3.46, 1.97] | 0.15 [0.49, 0.02] | -0.94 [-0.15, -1.03] | -0.16 [0.58, -0.31] | 0.96 [0.96, 0.82] |
| cp8kv | MD-OPLSAA-dryoct | 2.88 [3.25, 2.87] | 2.72 [3.02, 2.71] | -2.72 [-2.65, -2.89] | 0.24 [0.48, 0.19] | 0.78 [1.61, 0.57] | 0.59 [0.92, 0.52] | 0.12 [0.17, 0.08] |
| 5585v | Alchemical-CGenFF | 2.88 [3.40, 2.69] | 2.55 [3.02, 2.29] | 2.40 [3.02, 2.13] | 0.04 [0.73, 0.01] | -0.41 [0.18, -0.77] | -0.20 [0.15, -0.38] | 0.46 [0.69, 0.32] |
| j4nb3 | FOURVAR | 2.89 [3.46, 2.79] | 2.63 [3.41, 2.50] | 2.63 [3.41, 2.50] | 0.01 [0.57, 0.01] | 0.12 [1.16, -0.02] | 0.16 [0.59, 0.12] | 0.89 [1.04, 0.84] |
| hf4wj | MD/S-HI-GAFF-SPCE/MBAR/ | 3.28 [3.87, 3.14] | 3.04 [3.42, 2.90] | -3.04 [-2.57, -3.35] | 0.34 [0.89, 0.12] | 1.31 [1.59, 1.25] | 0.38 [0.71, 0.04] | 0.09 [0.16, 0.06] |
| pku5g | SAMPL5_49_retro3 | 4.87 [5.30, 4.33] | 4.68 [5.19, 4.15] | 4.68 [5.19, 4.15] | 0.49 [0.76, 0.08] | 1.80 [1.96, 0.60] | 0.56 [0.84, 0.27] | 0.39 [0.47, 0.32] |
| po4g2 | SAMPL5_49 | 5.46 [6.37, 5.16] | 5.17 [6.08, 4.83] | 5.17 [6.08, 4.83] | 0.51 [0.81, 0.22] | 2.33 [3.40, 1.77] | 0.56 [0.80, 0.24] | 0.34 [0.50, 0.28] |

Notes

- RMSE: Root mean square error
- MAE: Mean absolute error
- ME: Mean error
- R2: R-squared, square of Pearson correlation coefficient
- m: slope of the line fit to predicted vs experimental logP values
- ES: error slope calculated from the QQ Plots of model uncertainty predictions
- Mean and 95% confidence intervals of RMSE, MAE, ME, R2, and m were calculated by bootstrapping with 10000 samples.
- 95% confidence intervals of ES were calculated by bootstrapping with 1000 samples.