

Supplementary materials for Theoretical design and prediction of properties for dinitromethyl, fluorodinitromethyl, and (difluoroamino)dinitromethyl derivatives of triazole and tetrazole

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Summary of surface analysis of compound **A1-L3**.

Compound **A1**:

Volume: 1161.01720 Bohr³ (172.04504 Angstrom³)
Minimal value: -26.45030 kcal/mol Maximal value: 67.75952 kcal/mol
Overall surface area: 632.33664 Bohr² (177.07232 Angstrom²)
Positive surface area: 262.57808 Bohr² (73.52936 Angstrom²)
Negative surface area: 369.75856 Bohr² (103.54296 Angstrom²)
Overall average value: 0.00286700 a.u. (1.79907 kcal/mol)
Positive average value: 0.03948180 a.u. (24.77522 kcal/mol)
Negative average value: -0.02313441 a.u. (-14.51708 kcal/mol)
Overall variance (σ^2_{tot}): 0.00080571 a.u.² (317.26410 (kcal/mol)²)
Positive variance: 0.00070111 a.u.² (276.07444 (kcal/mol)²)
Negative variance: 0.00010460 a.u.² (41.18967 (kcal/mol)²)
Balance of charges (μ): 0.11297246
Product of σ^2_{tot} and μ : 0.00009102 a.u.² (35.84211 (kcal/mol)²)
Internal charge separation (Π): 0.03046271 a.u. (19.11565 kcal/mol)

Compound **A2**:

Volume: 1191.86206 Bohr³ (176.61577 Angstrom³)
Minimal value: -23.50527 kcal/mol Maximal value: 70.14863 kcal/mol
Overall surface area: 641.60188 Bohr² (179.66685 Angstrom²)
Positive surface area: 232.91778 Bohr² (65.22363 Angstrom²)
Negative surface area: 408.68410 Bohr² (114.44322 Angstrom²)
Overall average value: 0.00190395 a.u. (1.19475 kcal/mol)

Positive average value: 0.04080176 a.u. (25.60351 kcal/mol)
Negative average value: -0.02026475 a.u. (-12.71633 kcal/mol)
Overall variance (σ^2_{tot}): 0.00094696 a.u.² (372.88313 (kcal/mol)²)
Positive variance: 0.00086306 a.u.² (339.84471 (kcal/mol)²)
Negative variance: 0.00008390 a.u.² (33.03842 (kcal/mol)²)
Balance of charges (μ): 0.08075218
Product of σ^2_{tot} and μ : 0.00007647 a.u.² (30.11113 (kcal/mol)²)
Internal charge separation (Π): 0.02826961 a.u. (17.73946 kcal/mol)

Compound **A3**:

Volume: 1335.30482 Bohr³ (197.87180 Angstrom³)
Minimal value: -22.10728 kcal/mol Maximal value: 70.77745 kcal/mol
Overall surface area: 690.82478 Bohr² (193.45067 Angstrom²)
Positive surface area: 223.27361 Bohr² (62.52299 Angstrom²)
Negative surface area: 467.55117 Bohr² (130.92768 Angstrom²)
Overall average value: 0.00103967 a.u. (0.65240 kcal/mol)
Positive average value: 0.04140923 a.u. (25.98471 kcal/mol)
Negative average value: -0.01823834 a.u. (-11.44474 kcal/mol)
Overall variance (σ^2_{tot}): 0.00100650 a.u.² (396.32794 (kcal/mol)²)
Positive variance: 0.00092357 a.u.² (363.67121 (kcal/mol)²)
Negative variance: 0.00008293 a.u.² (32.65673 (kcal/mol)²)
Balance of charges (μ): 0.07560879
Product of σ^2_{tot} and μ : 0.00007610 a.u.² (29.96587 (kcal/mol)²)
Internal charge separation (Π): 0.02610422 a.u. (16.38066 kcal/mol)

Compound **B1**:

Volume: 1368.87434 Bohr³ (202.84629 Angstrom³)
Minimal value: -26.54356 kcal/mol Maximal value: 56.70601 kcal/mol
Overall surface area: 734.75033 Bohr² (205.75108 Angstrom²)
Positive surface area: 426.70999 Bohr² (119.49098 Angstrom²)
Negative surface area: 308.04034 Bohr² (86.26009 Angstrom²)
Overall average value: 0.01067358 a.u. (6.69778 kcal/mol)
Positive average value: 0.03122336 a.u. (19.59297 kcal/mol)
Negative average value: -0.01779281 a.u. (-11.16517 kcal/mol)
Overall variance (σ^2_{tot}): 0.00066545 a.u.² (262.03487 (kcal/mol)²)
Positive variance: 0.00050758 a.u.² (199.86729 (kcal/mol)²)
Negative variance: 0.00015788 a.u.² (62.16759 (kcal/mol)²)
Balance of charges (μ): 0.18096206
Product of σ^2_{tot} and μ : 0.00012042 a.u.² (47.41837 (kcal/mol)²)
Internal charge separation (Π): 0.02541032 a.u. (15.94523 kcal/mol)

Compound B2

Volume: 1399.71976 Bohr³ (207.41711 Angstrom³)
Minimal value: -24.92730 kcal/mol Maximal value: 54.49913 kcal/mol
Overall surface area: 744.25558 Bohr² (208.41282 Angstrom²)
Positive surface area: 458.39867 Bohr² (128.36472 Angstrom²)
Negative surface area: 285.85691 Bohr² (80.04810 Angstrom²)
Overall average value: 0.00961748 a.u. (6.03507 kcal/mol)
Positive average value: 0.02667397 a.u. (16.73818 kcal/mol)
Negative average value: -0.01773421 a.u. (-11.12840 kcal/mol)
Overall variance (sigma²_tot): 0.00056206 a.u.² (221.32344 (kcal/mol)²)
Positive variance: 0.00040244 a.u.² (158.46759 (kcal/mol)²)
Negative variance: 0.00015963 a.u.² (62.85585 (kcal/mol)²)
Balance of charges (miu): 0.20334399
Product of sigma²_tot and miu: 0.00011429 a.u.² (45.00479 (kcal/mol)²)
Internal charge separation (Pi): 0.02247812 a.u. (14.10524 kcal/mol)

Compound B3

Volume: 1544.99237 Bohr³ (28.94430 Angstrom³)
Minimal value: -24.47646 kcal/mol Maximal value: 57.98739 kcal/mol
Overall surface area: 795.38440 Bohr² (222.73035 Angstrom²)
Positive surface area: 506.77113 Bohr² (141.91039 Angstrom²)
Negative surface area: 288.61327 Bohr² (80.81996 Angstrom²)
Overall average value: 0.00847222 a.u. (5.31640 kcal/mol)
Positive average value: 0.02320050 a.u. (14.55855 kcal/mol)
Negative average value: -0.01738893 a.u. (-10.91173 kcal/mol)
Overall variance (sigma²_tot): 0.00050672 a.u.² (199.53168 (kcal/mol)²)
Positive variance: 0.00036368 a.u.² (143.20711 (kcal/mol)²)
Negative variance: 0.00014304 a.u.² (56.32457 (kcal/mol)²)
Balance of charges (miu): 0.20259967
Product of sigma²_tot and miu: 0.00010266 a.u.² (40.42505 (kcal/mol)²)
Internal charge separation (Pi): 0.02005137 a.u. (12.58244 kcal/mol)

Compound C1

Volume: 1571.17344 Bohr³ (232.82393 Angstrom³)
Minimal value: -20.33961 kcal/mol Maximal value: 60.21282 kcal/mol
Overall surface area: 826.47460 Bohr² (231.43649 Angstrom²)
Positive surface area: 446.88025 Bohr² (125.13923 Angstrom²)
Negative surface area: 379.59435 Bohr² (106.29726 Angstrom²)
Overall average value: 0.01130688 a.u. (7.09518 kcal/mol)

Positive average value: 0.03164944 a.u. (19.86034 kcal/mol)
Negative average value: -0.01264154 a.u. (-7.93269 kcal/mol)
Overall variance (σ^2_{tot}): 0.00068192 a.u.² (268.51777 (kcal/mol)²)
Positive variance: 0.00061337 a.u.² (241.52649 (kcal/mol)²)
Negative variance: 0.00006855 a.u.² (26.99128 (kcal/mol)²)
Balance of charges (μ): 0.09041536
Product of σ^2_{tot} and μ : 0.00006166 a.u.² (24.27813 (kcal/mol)²)
Internal charge separation (Π): 0.02381712 a.u. (14.94548 kcal/mol)

Compound C2

Volume: 1596.69885 Bohr³ (236.60641 Angstrom³)
Minimal value: -18.74713 kcal/mol Maximal value: 56.76213 kcal/mol
Overall surface area: 825.67598 Bohr² (231.21286 Angstrom²)
Positive surface area: 456.87361 Bohr² (127.93766 Angstrom²)
Negative surface area: 368.80236 Bohr² (103.27519 Angstrom²)
Overall average value: 0.00995679 a.u. (6.24799 kcal/mol)
Positive average value: 0.02708322 a.u. (16.99499 kcal/mol)
Negative average value: -0.01125949 a.u. (-7.06544 kcal/mol)
Overall variance (σ^2_{tot}): 0.00055007 a.u.² (216.60105 (kcal/mol)²)
Positive variance: 0.00049265 a.u.² (193.98846 (kcal/mol)²)
Negative variance: 0.00005743 a.u.² (22.61259 (kcal/mol)²)
Balance of charges (μ): 0.09349861
Product of σ^2_{tot} and μ : 0.00005143 a.u.² (20.25190 (kcal/mol)²)
Internal charge separation (Π): 0.02055084 a.u. (12.89586 kcal/mol)

Compound C3

Volume: 1737.65571 Bohr³ (257.49407 Angstrom³)
Minimal value: -18.67240 kcal/mol Maximal value: 52.53153 kcal/mol
Overall surface area: 869.86795 Bohr² (243.58787 Angstrom²)
Positive surface area: 520.92745 Bohr² (145.87457 Angstrom²)
Negative surface area: 348.94050 Bohr² (97.71331 Angstrom²)
Overall average value: 0.00928080 a.u. (5.82379 kcal/mol)
Positive average value 0.02325947 a.u. (14.59555 kcal/mol)
Negative average value: -0.01158773 a.u. (-7.27142 kcal/mol)
Overall variance (σ^2_{tot}): 0.00048163 a.u.² (189.65241 (kcal/mol)²)
Positive variance: 0.00041943 a.u.² (165.15976 (kcal/mol)²)
Negative variance: 0.00006220 a.u.² (24.49266 (kcal/mol)²)
Balance of charges (μ): 0.11246655
Product of σ^2_{tot} and μ : 0.00005417 a.u.² (21.32955 (kcal/mol)²)
Internal charge separation (Π): 0.01853816 a.u. (11.63288 kcal/mol)

Compound D1

Volume: 1739.38930 Bohr³ (257.75096 Angstrom³)
Minimal value: -21.90071 kcal/mol Maximal value: 82.25389 kcal/mol
Overall surface area: 907.47690 Bohr² (254.11945 Angstrom²)
Positive surface area: 401.56262 Bohr² (112.44900 Angstrom²)
Negative surface area: 505.91428 Bohr² (141.67045 Angstrom²)
Overall average value: 0.00895013 a.u. (5.61629 kcal/mol)
Positive average value: 0.03920098 a.u. (24.59901 kcal/mol)
Negative average value: -0.01506108 a.u. (-9.45098 kcal/mol)
Overall variance (sigma²_{tot}): 0.00122666 a.u.² 483.01918 (kcal/mol)²)
Positive variance: 0.00116032 a.u.² (456.89762 (kcal/mol)²)
Negative variance: 0.00006634 a.u.² (6.12157 (kcal/mol)²)
Balance of charges (miu): 0.05115515
Product of sigma²_{tot} and miu: 0.00006275 a.u.² (24.70892 (kcal/mol)²)
Internal charge separation (Pi): 0.02764588 a.u. (17.34806 kcal/mol)

Compound D2

Volume: 1802.42650 Bohr³ 267.09211 Angstrom³)
Minimal value: -18.47766 kcal/mol Maximal value: 80.22234 kcal/mol
Overall surface area: 928.74545 Bohr² (260.07525 Angstrom²)
Positive surface area: 438.60236 Bohr² (122.82119 Angstrom²)
Negative surface area: 490.14309 Bohr² (137.25406 Angstrom²)
Overall average value: 0.00805471 a.u. (5.05441 kcal/mol)
Positive average value: 0.03055683 a.u. (19.17472 kcal/mol)
Negative average value: -0.01208121 a.u. (-7.58108 kcal/mol)
Overall variance (sigma²_{tot}): 0.00090311 a.u.² (355.61515 (kcal/mol)²)
Positive variance: 0.00085564 a.u.² (336.92295 (kcal/mol)²)
Negative variance: 0.00004747 a.u.² (18.69220 (kcal/mol)²)
Balance of charges (miu): 0.04980014
Product of sigma²_{tot} and miu: 0.00004497 a.u.² (17.70969 (kcal/mol)²)
Internal charge separation (Pi): 0.02231370 a.u. (14.00207 kcal/mol)

Compound D3

Volume: 2085.47121 Bohr³ (309.03502 Angstrom³)
Minimal value: -17.01240 kcal/mol Maximal value: 71.61833 kcal/mol
Overall surface area: 1022.26611 Bohr² (286.26371 Angstrom²)
Positive surface area: 551.24128 Bohr² (154.36330 Angstrom²)
Negative surface area: 471.02483 Bohr² (131.90041 Angstrom²)
Overall average value: 0.00692987 a.u. (4.34856 kcal/mol)

Positive average value: 0.02240397 a.u. (14.05872 kcal/mol)
Negative average value: -0.01117951 a.u. (-7.01525 kcal/mol)
Overall variance (σ^2_{tot}): 0.00055576 a.u.² (218.84027 (kcal/mol)²)
Positive variance: 0.00050542 a.u.² (199.01922 (kcal/mol)²)
Negative variance: 0.00005034 a.u.² (19.82105 (kcal/mol)²)
Balance of charges (μ): 0.08236963
Product of σ^2_{tot} and μ : 0.00004578 a.u.² (18.02579 (kcal/mol)²)
Internal charge separation (Π): 0.01774918 a.u. (11.13779 kcal/mol)

Compound E1

Volume: 1167.34914 Bohr³ (172.98333 Angstrom³)
Minimal value: -30.80524 kcal/mol Maximal value: 60.10208 kcal/mol
Overall surface area: 633.77813 Bohr² (177.47598 Angstrom²)
Positive surface area: 287.00135 Bohr² (80.36858 Angstrom²)
Negative surface area: 346.77678 Bohr² (97.10740 Angstrom²)
Overall average value: 0.00604819 a.u. (3.79530 kcal/mol)
Positive average value: 0.03832912 a.u. (24.05190 kcal/mol)
Negative average value: -0.02066832 a.u. (-12.96958 kcal/mol)
Overall variance (σ^2_{tot}): 0.00078629 a.u.² (309.61656 (kcal/mol)²)
Positive variance: 0.00067520 a.u.² (265.87251 (kcal/mol)²)
Negative variance: 0.00011109 a.u.² (43.74406 (kcal/mol)²)
Balance of charges (μ): 0.12132327
Product of σ^2_{tot} and μ : 0.00009540 a.u.² (37.56369 (kcal/mol)²)
Internal charge separation (Π): 0.02951241 a.u. (18.51933 kcal/mol)

Compound E2

Volume: 1198.23869 Bohr³ (177.56069 Angstrom³)
Minimal value: -27.69761 kcal/mol Maximal value: 56.22691 kcal/mol
Overall surface area: 642.42671 Bohr² (179.89783 Angstrom²)
Positive surface area: 305.72488 Bohr² (85.61170 Angstrom²)
Negative surface area: 336.70183 Bohr² (94.28613 Angstrom²)
Overall average value: 0.00532900 a.u. (3.34400 kcal/mol)
Positive average value: 0.02986322 a.u. (18.73947 kcal/mol)
Negative average value: -0.01694804 a.u. (-10.63507 kcal/mol)
Overall variance (σ^2_{tot}): 0.00051471 a.u.² (202.67526 (kcal/mol)²)
Positive variance: 0.00042974 a.u.² (169.21827 (kcal/mol)²)
Negative variance: 0.00008497 a.u.² (33.45699 (kcal/mol)²)
Balance of charges (μ): 0.13782648
Product of σ^2_{tot} and μ : 0.00007094 a.u.² (27.93402 (kcal/mol)²)
Internal charge separation (Π): 0.02362214 a.u. (14.82313 kcal/mol)

Compound E3

Volume: 1343.24183 Bohr³ (199.04795 Angstrom³)
Minimal value: -26.73982 kcal/mol Maximal value: 50.27644 kcal/mol
Overall surface area: 690.56569 Bohr² (193.37812 Angstrom²)
Positive surface area: 344.84911 Bohr² (96.56760 Angstrom²)
Negative surface area: 345.71658 Bohr² (96.81052 Angstrom²)
Overall average value: 0.00473418 a.u. (2.97074 kcal/mol)
Positive average value: 0.02499066 a.u. (15.68189 kcal/mol)
Negative average value: -0.01547148 a.u. (-9.70851 kcal/mol)
Overall variance (sigma²_{tot}): 0.00049219 a.u.² (193.81037 (kcal/mol)²)
Positive variance: 0.00041442 a.u.² (163.18754 (kcal/mol)²)
Negative variance: 0.00007777 a.u.² (30.62283 (kcal/mol)²)
Balance of charges (miu): 0.13303879
Product of sigma²_{tot} and miu: 0.00006548 a.u.² (25.78430 (kcal/mol)²)
Internal charge separation (Pi): 0.02062411 a.u. (12.94184 kcal/mol)

Compound F1

Volume: 1374.86423 Bohr³ (203.73390 Angstrom³)
Minimal value: -25.76206 kcal/mol Maximal value: 71.17432 kcal/mol
Overall surface area: 737.95779 Bohr² (206.64926 Angstrom²)
Positive surface area: 356.57397 Bohr² (99.85090 Angstrom²)
Negative surface area: 381.38381 Bohr² (106.79836 Angstrom²)
Overall average value: 0.01056237 a.u. (6.62800 kcal/mol)
Positive average value: 0.03899966 a.u. (24.47268 kcal/mol)
Negative average value: -0.01602501 a.u. (-10.05585 kcal/mol)
Overall variance (sigma²_{tot}): 0.00106955 a.u.² (421.15414 (kcal/mol)²)
Positive variance: 0.00095989 a.u.² (377.97423 (kcal/mol)²)
Negative variance: 0.00010966 a.u.² (43.17991 (kcal/mol)²)
Balance of charges (miu): 0.09201566
Product of sigma²_{tot} and miu: 0.00009842 a.u.² (38.75278 (kcal/mol)²)
Internal charge separation (Pi): 0.02871587 a.u. (18.01950 kcal/mol)

Compound F2

Volume: 1374.86423 Bohr³ (203.73390 Angstrom³)
Minimal value: -23.13961 kcal/mol Maximal value: 67.93967 kcal/mol
Overall surface area: 747.67051 Bohr² (209.36910 Angstrom²)
Positive surface area: 402.45674 Bohr² (112.69938 Angstrom²)
Negative surface area: 345.21377 Bohr² (96.66971 Angstrom²)
Overall average value: 0.01000278 a.u. (6.27685 kcal/mol)

Positive average value: 0.03055933 a.u. (19.17628 kcal/mol)
Negative average value: -0.01396243 a.u. (-8.76156 kcal/mol)
Overall variance (σ^2_{tot}): 0.00065837 a.u.² (259.24552 (kcal/mol)²)
Positive variance: 0.00055224 a.u.² (217.45406 (kcal/mol)²)
Negative variance: 0.00010613 a.u.² (41.79145 (kcal/mol)²)
Balance of charges (μ): 0.13521738
Product of σ^2_{tot} and μ : 0.00008902 a.u.² (35.05450 (kcal/mol)²)
Internal charge separation (Π): 0.02350185 a.u. (14.74765 kcal/mol)

Compound F2

Volume: 1406.92653 Bohr³ (208.48505 Angstrom³)
Minimal value: -23.13961 kcal/mol Maximal value: 67.93967 kcal/mol
Overall surface area: 747.67051 Bohr² (209.36910 Angstrom²)
Positive surface area: 402.45674 Bohr² (112.69938 Angstrom²)
Negative surface area: 345.21377 Bohr² (96.66971 Angstrom²)
Overall average value: 0.01000278 a.u. (6.27685 kcal/mol)
Positive average value: 0.03055933 a.u. (19.17628 kcal/mol)
Negative average value: -0.01396243 a.u. (-8.76156 kcal/mol)
Overall variance (σ^2_{tot}): 0.00065837 a.u.² (259.24552 (kcal/mol)²)
Positive variance: 0.00055224 a.u.² (217.45406 (kcal/mol)²)
Negative variance: 0.00010613 a.u.² (41.79145 (kcal/mol)²)
Balance of charges (μ): 0.13521738
Product of σ^2_{tot} and μ : 0.00008902 a.u.² (35.05450 (kcal/mol)²)
Internal charge separation (Π): 0.02350185 a.u. (14.74765 kcal/mol)

Compound F3

Volume: 1551.99944 Bohr³ (229.98264 Angstrom³)
Minimal value: -22.58921 kcal/mol Maximal value: 61.22908 kcal/mol
Overall surface area: 796.05794 Bohr² (222.91896 Angstrom²)
Positive surface area: 463.14094 Bohr² (129.69269 Angstrom²)
Negative surface area: 332.91700 Bohr² (93.22627 Angstrom²)
Overall average value: 0.00938405 a.u. (5.88858 kcal/mol)
Positive average value: 0.02587755 a.u. (16.23842 kcal/mol)
Negative average value: -0.01356106 a.u. (-8.50970 kcal/mol)
Overall variance (σ^2_{tot}): 0.00054297 a.u.² (213.80394 (kcal/mol)²)
Positive variance: 0.00043362 a.u.² (170.74520 (kcal/mol)²)
Negative variance: 0.00010935 a.u.² (43.05874 (kcal/mol)²)
Balance of charges (μ): 0.16083422
Product of σ^2_{tot} and μ : 0.00008733 a.u.² (34.38699 (kcal/mol)²)
Internal charge separation (Π): 0.02051324 a.u. (12.87226 kcal/mol)

Compound G1

Volume: 1584.31971 Bohr³ (234.77201 Angstrom³)
Minimal value: -18.55578 kcal/mol Maximal value: 59.05282 kcal/mol
Overall surface area: 839.73836 Bohr² (235.15073 Angstrom²)
Positive surface area: 454.62312 Bohr² (127.30746 Angstrom²)
Negative surface area: 385.11524 Bohr² (107.84327 Angstrom²)
Overall average value: 0.01091940 a.u. (6.85204 kcal/mol)
Positive average value: 0.03062378 a.u. (19.21673 kcal/mol)
Negative average value: -0.01234133 a.u. (-7.74431 kcal/mol)
Overall variance (sigma²_{tot}): 0.00065153 a.u.² (256.55070 (kcal/mol)²)
Positive variance: 0.00059424 a.u.² (233.99341 (kcal/mol)²)
Negative variance: 0.00005729 a.u.² (22.55730 (kcal/mol)²)
Balance of charges (miu): 0.08019445
Product of sigma²_{tot} and miu: 0.00005225 a.u.² (20.57394 (kcal/mol)²)
Internal charge separation (Pi): 0.02311990 a.u. (14.50797 kcal/mol)

Compound G2

Volume: 1616.61807 Bohr³ (239.55813 Angstrom³)
Minimal value: -17.07844 kcal/mol Maximal value: 51.59745 kcal/mol
Overall surface area: 849.38035 Bohr² (237.85076 Angstrom²)
Positive surface area: 506.97741 Bohr² (141.96815 Angstrom²)
Negative surface area: 342.40294 Bohr² (95.88260 Angstrom²)
Overall average value: 0.01028762 a.u. (6.45558 kcal/mol)
Positive average value: 0.02478678 a.u. (15.55395 kcal/mol)
Negative average value: -0.01118051 a.u. (-7.01588 kcal/mol)
Overall variance (sigma²_{tot}): 0.00041524 a.u.² (163.51022 (kcal/mol)²)
Positive variance: 0.00036218 a.u.² (142.61674 (kcal/mol)²)
Negative variance: 0.00005306 a.u.² (20.89348 (kcal/mol)²)
Balance of charges (miu): 0.11145293
Product of sigma²_{tot} and miu: 0.00004628 a.u.² (18.22369 (kcal/mol)²)
Internal charge separation (Pi): 0.01924284 a.u. (12.07508 kcal/mol)

Compound G3

Volume: 1761.74741 Bohr³ (261.06409 Angstrom³)
Minimal value: -17.14640 kcal/mol Maximal value: 47.35644 kcal/mol
Overall surface area: 899.29516 Bohr² (251.82833 Angstrom²)
Positive surface area: 573.95080 Bohr² (160.72262 Angstrom²)
Negative surface area: 325.34436 Bohr² (91.10571 Angstrom²)
Overall average value: 0.00945039 a.u. (5.93021 kcal/mol)

Positive average value: 0.02130011 a.u. (13.36603 kcal/mol)
Negative average value: -0.01145409 a.u. (-7.18756 kcal/mol)
Overall variance (σ^2_{tot}): 0.00033029 a.u.² (130.05896 (kcal/mol)²)
Positive variance: 0.00027556 a.u.² (108.50881 (kcal/mol)²)
Negative variance: 0.00005473 a.u.² (21.55015 (kcal/mol)²)
Balance of charges (μ): 0.13824033
Product of σ^2_{tot} and μ : 0.00004566 a.u.² (17.97939 (kcal/mol)²)
Internal charge separation (Π): 0.01682531 a.u. (10.55805 kcal/mol)

Compound H1

Volume: 1720.27959 Bohr³ (254.91919 Angstrom³)
Minimal value: -25.04089 kcal/mol Maximal value: 74.72560 kcal/mol
Overall surface area: 860.80837 Bohr² (241.05093 Angstrom²)
Positive surface area: 406.95233 Bohr² (113.95828 Angstrom²)
Negative surface area: 453.85604 Bohr² (127.09265 Angstrom²)
Overall average value: 0.00702177 a.u. (4.40623 kcal/mol)
Positive average value: 0.03378920 a.u. (21.20306 kcal/mol)
Negative average value: -0.01697937 a.u. (-10.65472 kcal/mol)
Overall variance (σ^2_{tot}): 0.00079692 a.u.² (313.80356 (kcal/mol)²)
Positive variance: 0.00070669 a.u.² (278.27081 (kcal/mol)²)
Negative variance: 0.00009024 a.u.² (35.53275 (kcal/mol)²)
Balance of charges (μ): 0.10041088
Product of σ^2_{tot} and μ : 0.00008002 a.u.² (31.50929 (kcal/mol)²)
Internal charge separation (Π): 0.02585419 a.u. (16.22376 kcal/mol)

Compound H2

Volume: 1786.29451 Bohr³ (264.70159 Angstrom³)
Minimal value: -18.30467 kcal/mol Maximal value: 78.22352 kcal/mol
Overall surface area: 883.98380 Bohr² (247.54071 Angstrom²)
Positive surface area: 411.21605 Bohr² (115.15224 Angstrom²)
Negative surface area: 472.76775 Bohr² (132.38847 Angstrom²)
Overall average value: 0.00605803 a.u. (3.80148 kcal/mol)
Positive average value: 0.02746523 a.u. (17.23471 kcal/mol)
Negative average value: -0.01256207 a.u. (-7.88282 kcal/mol)
Overall variance (σ^2_{tot}): 0.00080846 a.u.² (318.34494 (kcal/mol)²)
Positive variance: 0.00076561 a.u.² (301.47365 (kcal/mol)²)
Negative variance: 0.00004285 a.u.² (16.87129 (kcal/mol)²)
Balance of charges (μ): 0.05018822
Product of σ^2_{tot} and μ : 0.00004057 a.u.² (15.97717 (kcal/mol)²)
Internal charge separation (Π): 0.02052967 a.u. (12.88257 kcal/mol)

Compound H3

Volume: 2055.71357 Bohr³ (304.62539 Angstrom³)
Minimal value: -18.42915 kcal/mol Maximal value: 79.30241 kcal/mol
Overall surface area: 955.64394 Bohr² (267.60760 Angstrom²)
Positive surface area: 439.19393 Bohr² (122.98684 Angstrom²)
Negative surface area: 516.45001 Bohr² (144.62075 Angstrom²)
Overall average value: 0.00469759 a.u. (2.94779 kcal/mol)
Positive average value: 0.02394732 a.u. (15.02718 kcal/mol)
Negative average value: -0.01167256 a.u. (-7.32465 kcal/mol)
Overall variance (σ^2_{tot}): 0.00083842 a.u.² (330.14200 (kcal/mol)²)
Positive variance: 0.00079309 a.u.² (312.29507 (kcal/mol)²)
Negative variance: 0.00004532 a.u.² (17.84692 (kcal/mol)²)
Balance of charges (μ): 0.05113602
Product of σ^2_{tot} and μ : 0.00004287 a.u.² (16.88215 (kcal/mol)²)
Internal charge separation (Π): 0.01820789 a.u. (11.42563 kcal/mol)

Compound I1

Volume: 1120.87653 Bohr³ (166.09680 Angstrom³)
Minimal value: -29.09904 kcal/mol Maximal value: 64.78201 kcal/mol
Overall surface area: 612.61281 Bohr² (171.54908 Angstrom²)
Positive surface area: 339.05583 Bohr² (94.94532 Angstrom²)
Negative surface area: 273.55698 Bohr² (76.60377 Angstrom²)
Overall average value: 0.01079038 a.u. (6.77107 kcal/mol)
Positive average value: 0.03196347 a.u. (20.05740 kcal/mol)
Negative average value: -0.01545226 a.u. (-9.69645 kcal/mol)
Overall variance (σ^2_{tot}): 0.00069294 a.u.² (272.85648 (kcal/mol)²)
Positive variance: 0.00056844 a.u.² (223.83425 (kcal/mol)²)
Negative variance: 0.00012449 a.u.² (49.02224 (kcal/mol)²)
Balance of charges (μ): 0.14738426
Product of σ^2_{tot} and μ : 0.00010213 a.u.² (40.21475 (kcal/mol)²)
Internal charge separation (Π): 0.02492051 a.u. (15.63787 kcal/mol)

Compound I2

Volume: 1149.91607 Bohr³ (170.40002 Angstrom³)
Minimal value: -28.16582 kcal/mol Maximal value: 66.62491 kcal/mol
Overall surface area: 621.43771 Bohr² (174.02031 Angstrom²)
Positive surface area: 351.10385 Bohr² (98.31911 Angstrom²)
Negative surface area: 270.33386 Bohr² (75.70120 Angstrom²)
Overall average value: 0.00984551 a.u. (6.17815 kcal/mol)

Positive average value: 0.02843881 a.u. (17.84564 kcal/mol)
Negative average value: -0.01430307 a.u. (-8.97532 kcal/mol)
Overall variance (σ^2_{tot}): 0.00072549 a.u.² (285.67581 (kcal/mol)²)
Positive variance: 0.00059382 a.u.² (233.82822 (kcal/mol)²)
Negative variance: 0.00013167 a.u.² (51.84759 (kcal/mol)²)
Balance of charges (μ): 0.14855201
Product of σ^2_{tot} and μ : 0.00010777 a.u.² (42.43772 (kcal/mol)²)
Internal charge separation (Π): 0.02283017 a.u. (14.32616 kcal/mol)

Compound I3

Volume: 1297.53003 Bohr³ (192.27415 Angstrom³)
Minimal value: -27.22581 kcal/mol Maximal value: 68.29879 kcal/mol
Overall surface area: 672.39225 Bohr² (188.28904 Angstrom²)
Positive surface area: 381.04489 Bohr² (106.70345 Angstrom²)
Negative surface area: 291.34737 Bohr² (81.58558 Angstrom²)
Overall average value: 0.00765293 a.u. (4.80229 kcal/mol)
Positive average value: 0.02420083 a.u. (15.18626 kcal/mol)
Negative average value: -0.01398959 a.u. (-8.77861 kcal/mol)
Overall variance (σ^2_{tot}): 0.00060687 a.u.² (238.96486 (kcal/mol)²)
Positive variance: 0.00050056 a.u.² (197.10568 (kcal/mol)²)
Negative variance: 0.00010630 a.u.² (41.85919 (kcal/mol)²)
Balance of charges (μ): 0.14448469
Product of σ^2_{tot} and μ : 0.00008768 a.u.² (34.52676 (kcal/mol)²)
Internal charge separation (Π): 0.01974156 a.u. (12.38802 kcal/mol)

Compound J1

Volume: 1341.74257 Bohr³ (198.82578 Angstrom³)
Minimal value: -18.36252 kcal/mol Maximal value: 48.30848 kcal/mol
Overall surface area: 728.70368 Bohr² (204.05784 Angstrom²)
Positive surface area: 366.97002 Bohr² (102.76209 Angstrom²)
Negative surface area: 361.73366 Bohr² (101.29576 Angstrom²)
Overall average value: 0.00839329 a.u. (5.26687 kcal/mol)
Positive average value: 0.02809882 a.u. (17.63229 kcal/mol)
Negative average value: -0.01159749 a.u. (-7.27754 kcal/mol)
Overall variance (σ^2_{tot}): 0.00052830 a.u.² (208.02772 (kcal/mol)²)
Positive variance: 0.00047308 a.u.² (186.28249 (kcal/mol)²)
Negative variance: 0.00005522 a.u.² (21.74523 (kcal/mol)²)
Balance of charges (μ): 0.09360384
Product of σ^2_{tot} and μ : 0.00004945 a.u.² (19.47219 (kcal/mol)²)
Internal charge separation (Π): 0.02093740 a.u. (13.13843 kcal/mol)

Compound J2

Volume: 1374.01494 Bohr³ (203.60805 Angstrom³)
Minimal value: -15.28528 kcal/mol Maximal value: 50.79181 kcal/mol
Overall surface area: 739.15636 Bohr² (206.98489 Angstrom²)
Positive surface area: 409.20645 Bohr² (114.58949 Angstrom²)
Negative surface area: 329.94990 Bohr² (92.39540 Angstrom²)
Overall average value: 0.00771555 a.u. (4.84158 kcal/mol)
Positive average value: 0.02223494 a.u. (13.95265 kcal/mol)
Negative average value: -0.01029152 a.u. (-6.45803 kcal/mol)
Overall variance (σ^2_{tot}): 0.00044545 a.u.² (175.40352 (kcal/mol)²)
Positive variance: 0.00040518 a.u.² (159.54834 (kcal/mol)²)
Negative variance: 0.00004027 a.u.² (15.85518 (kcal/mol)²)
Balance of charges (μ): 0.08222177
Product of σ^2_{tot} and μ : 0.00003663 a.u.² (14.42199 (kcal/mol)²)
Internal charge separation (Π): 0.01757357 a.u. (11.02759 kcal/mol)

Compound J3

Volume: 1517.51137 Bohr³ (224.87203 Angstrom³)
Minimal value: -14.30800 kcal/mol Maximal value: 50.60288 kcal/mol
Overall surface area: 788.16955 Bohr² (220.70998 Angstrom²)
Positive surface area: 448.71684 Bohr² (125.65353 Angstrom²)
Negative surface area: 339.45271 Bohr² (95.05645 Angstrom²)
Overall average value: 0.00693755 a.u. (4.35338 kcal/mol)
Positive average value: 0.01958419 a.u. (12.28928 kcal/mol)
Negative average value: -0.00977985 a.u. (-6.13695 kcal/mol)
Overall variance (σ^2_{tot}): 0.00041745 a.u.² (164.37804 (kcal/mol)²)
Positive variance: 0.00037957 a.u.² (149.46397 (kcal/mol)²)
Negative variance: 0.00003788 a.u.² (14.91407 (kcal/mol)²)
Balance of charges (μ): 0.08249833
Product of σ^2_{tot} and μ : 0.00003444 a.u.² (13.56091 (kcal/mol)²)
Internal charge separation (Π): 0.01588624 a.u. (9.96877 kcal/mol)

Compound K1

Volume: 1338.69852 Bohr³ (198.37470 Angstrom³)
Minimal value: -20.86834 kcal/mol Maximal value: 58.59120 kcal/mol
Overall surface area: 726.19851 Bohr² (203.35632 Angstrom²)
Positive surface area: 391.14216 Bohr² (109.53098 Angstrom²)
Negative surface area: 335.05635 Bohr² (93.82535 Angstrom²)
Overall average value: 0.00981361 a.u. (6.15814 kcal/mol)

Positive average value: 0.02989210 a.u. (18.75759 kcal/mol)
Negative average value: -0.01362587 a.u. (-8.55037 kcal/mol)
Overall variance (σ^2_{tot}): 0.00069267 a.u.² (272.75036 (kcal/mol)²)
Positive variance: 0.00060914 a.u.² (239.86154 (kcal/mol)²)
Negative variance: 0.00008352 a.u.² (32.88882 (kcal/mol)²)
Balance of charges (μ): 0.10604208
Product of σ^2_{tot} and μ : 0.00007345 a.u.² (28.92302 (kcal/mol)²)
Internal charge separation (Π): 0.02319924 a.u. (14.55775 kcal/mol)

Compound **K2**

Volume: 1371.25377 Bohr³ (203.19889 Angstrom³)
Minimal value: -19.36763 kcal/mol Maximal value: 52.29921 kcal/mol
Overall surface area: 736.01934 Bohr² (206.10644 Angstrom²)
Positive surface area: 436.69641 Bohr² (122.28747 Angstrom²)
Negative surface area: 299.32293 Bohr² (83.81897 Angstrom²)
Overall average value: 0.00909500 a.u. (5.70720 kcal/mol)
Positive average value: 0.02360724 a.u. (14.81378 kcal/mol)
Negative average value: -0.01207760 a.u. (-7.57881 kcal/mol)
Overall variance (σ^2_{tot}): 0.00042153 a.u.² (165.98493 (kcal/mol)²)
Positive variance: 0.00034467 a.u.² (135.71859 (kcal/mol)²)
Negative variance: 0.00007686 a.u.² (30.26634 (kcal/mol)²)
Balance of charges (μ): 0.14909461
Product of σ^2_{tot} and μ : 0.00006285 a.u.² (24.74746 (kcal/mol)²)
Internal charge separation (Π): 0.01882847 a.u. (11.81506 kcal/mol)

Compound **K3**

Volume: 1515.78486 Bohr³ (224.61619 Angstrom³)
Minimal value: -18.79059 kcal/mol Maximal value: 46.13483 kcal/mol
Overall surface area: 785.54086 Bohr² (219.97388 Angstrom²)
Positive surface area: 504.03437 Bohr² (141.14402 Angstrom²)
Negative surface area: 281.50649 Bohr² (78.82986 Angstrom²)
Overall average value: 0.00844874 a.u. (5.30167 kcal/mol)
Positive average value: 0.01971722 a.u. (12.37276 kcal/mol)
Negative average value: -0.01172735 a.u. (-7.35903 kcal/mol)
Overall variance (σ^2_{tot}): 0.00033843 a.u.² (133.26212 (kcal/mol)²)
Positive variance: 0.00026545 a.u.² (104.52405 (kcal/mol)²)
Negative variance: 0.00007298 a.u.² (28.73807 (kcal/mol)²)
Balance of charges (μ): 0.16914548
Product of σ^2_{tot} and μ : 0.00005724 a.u.² (22.54069 (kcal/mol)²)
Internal charge separation (Π): 0.01600867 a.u. (10.04560 kcal/mol)

Compound L1

Volume: 1707.05635 Bohr³ (252.95971 Angstrom³)
Minimal value: -17.89204 kcal/mol Maximal value: 56.83481 kcal/mol
Overall surface area: 895.69787 Bohr² (250.82099 Angstrom²)
Positive surface area: 459.66696 Bohr² (128.71988 Angstrom²)
Negative surface area: 436.03091 Bohr² (122.10111 Angstrom²)
Overall average value: 0.00904223 a.u. (5.67409 kcal/mol)
Positive average value: 0.02878748 a.u. (18.06443 kcal/mol)
Negative average value: -0.01177335 a.u. (-7.38790 kcal/mol)
Overall variance (σ^2_{tot}): 0.00064036 a.u.² (252.15302 (kcal/mol)²)
Positive variance: 0.00059159 a.u.² (232.94958 (kcal/mol)²)
Negative variance: 0.00004877 a.u.² (19.20344 (kcal/mol)²)
Balance of charges (μ): 0.07035784
Product of σ^2_{tot} and μ : 0.00004505 a.u.² (17.74094 (kcal/mol)²)
Internal charge separation (Π): 0.02161088 a.u. (13.56104 kcal/mol)

Compound L2

Volume: 1770.79273 Bohr³ (262.40447 Angstrom³)
Minimal value: -14.21131 kcal/mol Maximal value: 52.02280 kcal/mol
Overall surface area: 916.04352 Bohr² (256.51835 Angstrom²)
Positive surface area: 541.87395 Bohr² (151.74018 Angstrom²)
Negative surface area: 374.16958 Bohr² (104.77817 Angstrom²)
Overall average value: 0.00850555 a.u. (5.33732 kcal/mol)
Positive average value: 0.02043789 a.u. (12.82498 kcal/mol)
Negative average value: -0.00877491 a.u. (-5.50634 kcal/mol)
Overall variance (σ^2_{tot}): 0.00031561 a.u.² (124.27744 (kcal/mol)²)
Positive variance: 0.00028559 a.u.² (112.45801 (kcal/mol)²)
Negative variance: 0.00003002 a.u.² (11.81943 (kcal/mol)²)
Balance of charges (μ): 0.08606018
Product of σ^2_{tot} and μ : 0.00002716 a.u.² (10.69534 (kcal/mol)²)
Internal charge separation (Π): 0.01564214 a.u. (9.81560 kcal/mol)

Compound L3

Volume: 2059.19468 Bohr³ (305.14124 Angstrom³)
Minimal value: -13.21185 kcal/mol Maximal value: 43.20712 kcal/mol
Overall surface area: 1014.46848 Bohr² (284.08015 Angstrom²)
Positive surface area: 663.91297 Bohr² (185.91459 Angstrom²)
Negative surface area: 350.55551 Bohr² (98.16555 Angstrom²)
Overall average value: 0.00748878 a.u. (4.69928 kcal/mol)

Positive average value: 0.01573390 a.u. (9.87318 kcal/mol)
Negative average value: -0.00812655 a.u. (-5.09949 kcal/mol)
Overall variance (σ^2_{tot}): 0.00019290 a.u.² (75.95747 (kcal/mol)²)
Positive variance: 0.00016600 a.u.² (65.36404 (kcal/mol)²)
Negative variance: 0.00002690 a.u.² (10.59343 (kcal/mol)²)
Balance of charges (μ): 0.12001473
Product of σ^2_{tot} and μ : 0.00002315 a.u.² (9.11602 (kcal/mol)²)
Internal charge separation (Π): 0.01232453 a.u. (7.73377 kcal/mol)