

| | α_{Br} | α_{C} | α_{Cl} | α_{F} | α_{H} | α_{N} | α_{O} | α_{S} | β_{Br} | β_{C} | β_{Cl} | β_{F} | β_{H} | β_{N} | β_{O} | β_{S} | γ_{Br} | γ_{C} | γ_{Cl} | γ_{F} | γ_{H} | γ_{N} | γ_{O} | γ_{S} | K |
|----------------------|----------------------|---------------------|----------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|--------------------|---------------------|--------------------|--------------------|--------------------|--------------------|--------------------|----------------------|---------------------|----------------------|---------------------|---------------------|---------------------|---------------------|---------------------|------|
| α_{Br} | 5 | 3 | 1 | 2 | 1 | 4 | 4 | 3 | -5287 | -0 | -0 | -72 | -0 | -8 | -48 | -68 | -2 | 0 | 0 | -0 | 0 | 0 | 0 | 0 | 3 |
| α_{C} | 3 | 6 | 3 | 3 | 2 | 8 | 5 | 5 | -372 | -0 | -0 | -8 | 0 | 2 | 8 | 11 | -0 | -0 | -0 | -0 | 0 | 0 | 0 | 0 | 5 |
| α_{Cl} | 1 | 3 | 3 | 1 | 1 | 4 | 3 | 2 | 192 | 0 | -0 | -9 | 0 | 1 | 5 | 18 | 0 | 0 | -1 | -0 | 0 | 0 | 0 | 0 | 3 |
| α_{F} | 2 | 3 | 1 | 4 | 1 | 4 | 4 | 2 | -1570 | -0 | -0 | -275 | -0 | -16 | -98 | -110 | -0 | 0 | -0 | -0 | 0 | 0 | 0 | 0 | 3 |
| α_{H} | 1 | 2 | 1 | 1 | 2 | 4 | 2 | 2 | 54 | 0 | 0 | 8 | -0 | 3 | 12 | 17 | 0 | 0 | 0 | -0 | -0 | 0 | 0 | 0 | 3 |
| α_{N} | 4 | 8 | 4 | 4 | 4 | 12 | 8 | 8 | -839 | -0 | -0 | -43 | 0 | -4 | -21 | -27 | -0 | 0 | -0 | -0 | 0 | -0 | 0 | 0 | 8 |
| α_{O} | 4 | 5 | 3 | 4 | 2 | 8 | 8 | 5 | -2090 | -0 | -0 | -202 | -0 | -27 | -170 | -227 | -0 | 0 | -0 | -0 | 0 | 0 | -0 | 0 | 5 |
| α_{S} | 3 | 5 | 2 | 2 | 2 | 8 | 5 | 5 | -450 | -0 | 0 | 14 | 0 | -1 | -11 | -38 | -0 | 0 | 0 | 0 | 0 | 0 | 0 | -0 | 5 |
| β_{Br} | -5287 | -372 | 192 | -1570 | 54 | -839 | -2090 | -450 | 9646769 | 7 | 26 | 125238 | 2 | 18830 | 110772 | 157620 | 1941 | 1 | -199 | 84 | -54 | -7 | 9 | -52 | -289 |
| β_{C} | -0 | -0 | 0 | -0 | 0 | -0 | -0 | -0 | 7 | 0 | 0 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | -0 | -0 | -0 | -0 | -0 | -0 | 0 |
| β_{Cl} | -0 | -0 | -0 | -0 | 0 | -0 | -0 | 0 | 26 | 0 | 0 | 3 | 0 | 0 | 2 | 2 | 0 | -0 | 0 | 0 | -0 | -0 | -0 | -0 | 0 |
| β_{F} | -72 | -8 | -9 | -275 | 8 | -43 | -202 | 14 | 125238 | 1 | 3 | 48584 | 0 | 2222 | 12862 | 16540 | 10 | 0 | 7 | 17 | -1 | -2 | -4 | -14 | 0 |
| β_{H} | -0 | 0 | 0 | -0 | -0 | 0 | -0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -0 | -0 | 0 | 0 | -0 | 0 | -0 | 0 |
| β_{N} | -8 | 2 | 1 | -16 | 3 | -4 | -27 | -1 | 18830 | 0 | 0 | 2222 | 0 | 339 | 1841 | 2708 | 1 | -0 | -0 | -1 | -0 | -0 | -0 | -1 | 2 |
| β_{O} | -48 | 8 | 5 | -98 | 12 | -21 | -170 | -11 | 110772 | 1 | 2 | 12862 | 0 | 1841 | 12645 | 15048 | 5 | -0 | -2 | -1 | -1 | -1 | 1 | -4 | 11 |
| β_{S} | -68 | 11 | 18 | -110 | 17 | -27 | -227 | -38 | 157620 | 1 | 2 | 16540 | 0 | 2708 | 15048 | 40393 | 9 | 0 | -14 | -19 | -1 | -1 | -4 | -10 | 18 |
| γ_{Br} | -2 | -0 | 0 | -0 | 0 | -0 | -0 | -0 | 1941 | 0 | 0 | 10 | 0 | 1 | 5 | 9 | 1 | 0 | -0 | 0 | -0 | 0 | 0 | 0 | -0 |
| γ_{C} | 0 | -0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | -0 | 0 | -0 | -0 | -0 | 0 | 0 | 0 | -0 | -0 | -0 | 0 | -0 | 0 | 0 |
| γ_{Cl} | 0 | -0 | -1 | -0 | 0 | -0 | -0 | 0 | -199 | -0 | 0 | 7 | -0 | -0 | -2 | -14 | -0 | -0 | 0 | 0 | -0 | -0 | -0 | -0 | -0 |
| γ_{F} | -0 | -0 | -0 | -0 | -0 | -0 | -0 | 0 | 84 | -0 | 0 | 17 | 0 | -1 | -1 | -19 | 0 | -0 | 0 | 0 | 0 | -0 | 0 | -0 | -0 |
| γ_{H} | 0 | 0 | 0 | 0 | -0 | 0 | 0 | 0 | -54 | -0 | -0 | -1 | 0 | -0 | -1 | -1 | -0 | -0 | -0 | 0 | 0 | -0 | -0 | -0 | 0 |
| γ_{N} | 0 | 0 | 0 | 0 | 0 | -0 | 0 | 0 | -7 | -0 | -0 | -2 | -0 | -0 | -1 | -1 | 0 | 0 | -0 | -0 | -0 | 0 | 0 | 0 | 0 |
| γ_{O} | 0 | 0 | 0 | 0 | 0 | 0 | -0 | 0 | 9 | -0 | -0 | -4 | 0 | -0 | 1 | -4 | 0 | -0 | -0 | 0 | -0 | 0 | 0 | 0 | 0 |
| γ_{S} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -0 | -52 | -0 | -0 | -14 | -0 | -1 | -4 | -10 | 0 | 0 | -0 | -0 | -0 | 0 | 0 | 0 | 0 |
| K | 3 | 5 | 3 | 3 | 3 | 8 | 5 | 5 | -289 | 0 | 0 | 0 | 0 | 2 | 11 | 18 | -0 | 0 | -0 | -0 | 0 | 0 | 0 | 0 | 5 |

(kcal/mol)^2