

chemical sample	bp(C)	PTRI	H	k	electron af	ionization p	energy tota	area (A^2)	volume (μ	Δ (HOMO-L	Δ electron ionization p	energy total (Hartree)	
benzene.mm	80				8.321	12.801	-19.51	84.63	56.21	4.48	1.104	1.523	23.356
1-CB	132	958			8.322	12.143	-23.414	101.72	69.37	3.821	1.105	0.865	19.452
12-DCB	180	1055	5162	2.142	8.11	11.817	-27.312	117.67	83.61	3.707	0.893	0.539	15.554
13-DCB	172.5	1021	5235	1.403	8.129	11.998	-27.318	118.72	82.93	3.869	0.912	0.72	15.548
14-DCB	173	1029	5304	1.206	8.324	11.664	-27.315	118.78	82.7	3.34	1.107	0.386	15.551
123-TCB	218.5	1244	5477	3.009	7.797	11.747	-31.207	133.26	96.49	3.95	0.58	0.469	11.659
124-TCB	214	1206	5421	2.815	8.069	11.524	-31.213	134.63	96.73	3.455	0.852	0.246	11.653
135-TCB	208	1158	5177	4.16	7.675	11.999	-31.222	135.64	95.94	4.324	0.458	0.721	11.644
1234-TCB	254	1423	6115	1.419	7.777	11.494	-35.098	148.8	110.06	3.717	0.56	0.216	7.768
1235-TCB	246	1369	6000	1.437	7.704	11.454	-35.108	150.22	109.34	3.75	0.487	0.176	7.758
1245-TCB	243	1369	5985	1.525	7.93	11.278	-35.108	150.52	110.44	3.348	0.713	0	7.758
12345-PCB	276	1576	6756	5.891	7.563	11.291	-38.989	164.27	122.92	3.728	0.346	0.013	3.877
HCB		1776			7.217	11.305	-42.866	177.76	136.38	4.088	0	0.027	0
MIN					7.217	11.278	-42.866	84.63	56.21		0	0	0

chemical sample	bp(C)	PTR	H	k	electron af	ionization p	energy tot	area (A^2)	volume (l	Δ (HOMO-l	Δ electron	ionization p	energy total (Hartree)
phenol.mm					8.31	12.428	-24.126	91.92	61.01	4.118	1.031	1.156	19.473
2-CP	175.5	1002	4602	7.842	8.113	11.945	-28.028	108.77	74.26	3.832	0.834	0.673	15.571
3-CP	214	1203	6164	4.04	8.142	12.091	-28.031	108.96	74.43	3.949	0.863	0.819	15.568
4-CP	220	1203	6159	8.559	8.311	11.87	-28.029	109.07	73.65	3.559	1.032	0.598	15.57
23-DCP	206	1200	5455	2.449	7.832	11.765	-31.925	124.66	87.67	3.933	0.553	0.493	11.674
24-DCP	209.5	1189	5645	2.262	8.051	11.693	-31.93	125.78	87.49	3.642	0.772	0.421	11.669
25-DCP	211	1190	5476	1.393	8.094	11.563	-31.929	125.8	87.84	3.469	0.815	0.291	11.67
26-DCP	219	1228	5501	2.606	7.872	11.912	-31.929	124.74	87.07	4.04	0.593	0.64	11.67
34-DCP	245.5	1408	6640	4.642	8.063	11.662	-31.927	125.03	87.14	3.599	0.784	0.39	11.672
35-DCP	233	1395	6359	8.278	7.758	11.989	-31.935	125.92	87.07	4.231	0.479	0.717	11.664
234-TCP		1408	6241	9.82	7.757	11.658	-35.819	140.3	100.78	3.901	0.478	0.386	7.78
235-TCP	248.5	1367	6082	1.238	7.757	11.459	-35.827	141.66	101.21	3.702	0.478	0.187	7.772
236-TCP		1421	6131	1.422	7.832	11.503	-35.824	140.59	100.76	3.671	0.553	0.231	7.775
245-TCP		1392	6303	7.978	7.927	11.36	-35.825	141.68	101.11	3.433	0.648	0.088	7.774
246-TCP	246	1386	6139	1.176	7.669	11.616	-35.832	141.71	100.22	3.947	0.39	0.344	7.767
345-TCP		1643			7.696	11.585	-35.822	140.58	99.99	3.889	0.417	0.313	7.777
2345-TCP		1602	6928	4.478	7.563	11.36	-39.71	155.8	113.9	3.797	0.284	0.088	3.889
2346-TCP		1602	7098	2.973	7.562	11.362	-39.718	156.17	113.48	3.8	0.283	0.09	3.881
2356-TCP		1593	6806	5.998	7.639	11.272	-39.719	156.25	114.14	3.633	0.36	0	3.88
PCP	310	1817			7.279	11.286	-43.599	169.91	127.15	4.007	0	0.014	0
MIN					7.279	11.272	-43.599	91.92	61.01				