Electronic Supplementary Material (ESI) for CrystEngComm.

Mining the Cambridge Database for theoretical chemistry. Mi–LJC: A new set of Lennard–Jones–Coulomb atom–atom potentials for the computer simulation of organic condensed matter

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Experimental ΔH_s and lattice energy data for the 377–molecule data set (kJ·mol^{-1}). "CSD refcode" is the Cambridge Structural Database reference codes. E_{LJC} and E_{CLP} are lattice energies by LJC or CLP functional.

CSD refcode	ΔH_s	E_{LJC}	%Dev	E_{CLP}	%Dev	compound name
ACETAC03	66.4	64.7	2.6	67.4	–1.5	acetic acid
FORMAC01	60.2	56.5	6.3	56.1	6.9	formic acid
FUMAAC01	136.4	119.5	12.4	122.5	10.2	trans–butenedioic acid
GLURAC13	130.6	129.3	1	143.2	–9.6	glutaric acid
HIFKUC	87.1	88.4	–1.5	82.6	5.1	3–furancarboxylic acid
MALIAC13	109.2	107.4	1.7	109.2	0	cis–butenedioic acid maleic acid.
MALNAC16	109.2	107	2.1	123.3	–12.9	malonic acid
MEMALA01	115	118.7	–3.2	125.6	–9.2	methylmalonic acid
OXALAC08	95.2	99.8	–4.8	119.1	–25.1	oxalic acid anhydrous.
PRONAC	72.1	72.3	–0.2	77.6	–7.6	propionic acid
SUCACB18	122	117.1	4	129.5	–6.1	succinic acid
ADIPAC20	144.5	131.6	9	137	5.2	adipic acid
BENZAC20	91	94.9	–4.2	86.2	5.3	benzoic acid
CLBZAC02	110	101.3	7.9	99.2	9.8	2–chlorobenzoic acid
CLBZAP13	105	101.8	3.1	98.6	6.1	4–chlorobenzoic acid
COVJIG01	94.3	97	–2.8	90.2	4.4	3–fluorobenzoic acid
FBENZA02	94	99.2	–5.5	97.6	–3.8	2–fluorobenzoic acid
FURDCA	122.8	109.2	11.1	130.4	–6.1	furan–2,5–dicarboxylic
MCBZAC02	104	102.3	1.6	101.1	2.7	3–chlorobenzoic acid
PFBZAD15	93	91.8	1.3	87.6	5.9	4–fluorobenzoic acid
BENZDC11	142	134	5.7	133.7	5.8	isophthalic acid
OTOLIC02	96	97.8	–1.8	94.5	1.6	o–toluic acid
PHTHAC06	130	134.6	–3.5	138.4	–6.5	phthalic acid
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
PIMELA15	140	142.6	–1.8	155	–10.7	heptanedioic acid
PTOLIC01	99	93.3	5.7	93.9	5.2	p–toluic acid

TEPHTH14	146	140	4.1	132.1	9.5	terephthalic acid
DMBNZA11	99	99.1	–0.1	100.2	–1.2	2,6–dimethylbenzoic acid
DMBZAC01	105	100.9	3.9	99.9	4.9	2,3–dimethylbenzoic acid
RUVQAA	110	105.7	3.9	105.7	4	2,4,5–trimethylbenzoic
WIZJUL	104	102	1.9	105.1	–1.1	2,4–dimethylbenzoic acid
CINMAC	107	101.8	4.9	96.4	9.9	trans cinnamic acid
TMBZAC01	104	97.9	5.9	107.3	–3.2	2,4,6–trimethylbenzoic
TMEBZA	111	104.2	6.1	104	6.3	3,4,5–trimethylbenzoic
NAPACA12	112	113.8	–1.6	120.2	–7.3	1–naphthaleneacetic
NAPOAC01	115.4	108.3	6.2	108.5	6	1–naphthoic acid
PEYGEF01	124	122.9	0.9	131.3	–5.9	2–naphthaleneacetic
NAPHAC02	118.4	112.5	5	108.2	8.6	2–naphthoic acid
ISENUP	113	105.6	6.6	110.3	2.4	octanoic
SUBRAC12	148	149.5	–1	152	–2.7	octanedioic
QQQFDJ01	122.1	135.5	–11	136.5	–11.8	9–anthracenecarboxylic
DCLPHM01	87	88.1	–1.3	100.1	–15	3,4–dichlorophenol
DNOPHL02	104.3	103.3	0.9	115.1	–10.3	2,4–dinitrophenol
DNPHOL02	112.3	105.5	6.1	122.9	–9.4	2,6–dinitrophenol
LETFEV	73	78.5	–7.5	91.7	–25.6	3,5–diFluorophenol
NITPOL08	95	94.5	0.5	94	1	4–nitrophenol
NTCPOL01	88	87.2	0.9	90.5	–2.9	4–chloro–2–nitrophenol
ONITPH	73	77	–5.4	87.8	–20.3	2–nitrophenol
PBRPOL	85	84.4	0.7	90.3	–6.2	4–bromophenol
PCPHOL01	93.2	107.9	–15.8	117.1	–25.7	pentachlorophenol
QQQBNG01	74	78.2	–5.7	75.5	–2	4–Fluorophenol
SILGOK	82.7	83.9	–1.4	92.6	–11.9	2,4,6–trichlorophenol
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
TEMWUD	74.5	79.8	–7.2	95.7	–28.5	2–nitro–1,3–dihydroxybenzene
UCAYED01	67.2	79.7	–18.6	88.9	–32.4	pentaFluorophenol
AMPHOL01	108	103.2	4.5	111.9	–3.6	4–aminophenol
AMPHOM02	101	96.9	4.1	99.9	1.1	2–aminophenol
BESKAL	130	123.4	5.1	151	–16.1	2,5–dihydroxybenzoic acid
BIDLOP02	123	123	0	121	1.6	3–hydroxybenzoic acid
CACDAM01	111	112	–0.9	135.2	–21.8	2,3–dihydroxybenzoic acid
CATCOL16	85	96.1	–13	114.1	–34.3	1,2–dihydroxybenzene
FECCOF01	110	125.6	–14.2	132.4	–20.4	1,6–hexanediol
HYQUIN08	100.4	111.2	–10.7	108.3	–7.8	1,4–dihydroxybenzene
LEZJAB01	109	115.2	–5.7	132.4	–21.5	2,6–dihydroxybenzoic acid
MAMPOL	104	95.1	8.5	104.7	–0.7	3–aminophenol
PHBALD11	101	90.7	10.2	107.6	–6.5	4–hydroxybenzaldehyde
PHGLOL01	134	130.7	2.4	160.8	–20	1,3,5–trihydroxybenzene
RESORA03	93	105.7	–13.6	113.5	–22	1,3–dihydroxybenzene
SALIAC19	97	95.4	1.6	108	–11.3	2–hydroxybenzoic acid
XAYCIJ	100	88.2	11.8	110.6	–10.6	3–hydroxybenzaldehyde

YELRIR	89	89.6	–0.7	95.1	–6.9	2–methyl–3–hydroxypyridine
ZZZEEU04	125	129.5	–3.6	145.9	–16.7	2,4–dihydroxybenzoic acid
DIMEDO02	100	103.2	–3.2	122.8	–22.8	5,5–dimethyl–1,3–cyclohexanedione
DIMPHE12	84.1	85.1	–1.1	102.3	–21.7	2,3–dimethylphenol
DMEPOL10	75.5	77.5	–2.7	90.1	–19.3	2,6–dimethylphenol
DMPHOL11	85.1	83	2.5	91.8	–7.8	2,5–dimethylphenol
HACTPH16	96.7	100.1	–3.4	123.4	–27.6	4–hydroxyacetophenone
SALMID02	101	98.8	2.1	110.6	–9.5	2–hydroxybenzamide
VIDMAX	125	124.7	0.2	142.1	–13.7	4–hydroxybenzamide
FAMDIG	112	93.6	16.4	104.2	6.9	5–chloro–8–hydroxyquinoline
FESNOG02	172.3	167	3.1	193	–12	3,4–dihydroxycinnamic acid caffeic acid
HEGFAB	116	116.8	–0.7	137.1	–18.2	1,3–dihydroxynaphthalene
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
HXQUIN11	89	84.5	5	98.7	–10.8	8–hydroxyquinoline
IPMEPL	91	85.8	5.8	95.6	–5.1	2–isopropyl–5–methylphenol thymol
NAPHOL01	90	93.5	–3.9	103.3	–14.8	1–naphthol
XAXSIY	90	85.3	5.2	98.4	–9.3	2,4,6–trimethylphenol
BOPSAA10	110	114.9	–4.4	128.9	–17.2	4–hydroxybiphenyl
DOHDPH02	143	145.2	–1.6	169.9	–18.8	4,4' –dihydroxybiphenyl
NUTSUQ	114	120.8	–5.9	122.8	–7.7	2,2' –dihydroxybiphenyl
ACEMID05	79	79.3	–0.3	78.4	0.8	acetamide
APYFEB01	113	108.8	3.7	88.3	21.9	tetrahydro–2–pyrimidone
ARCLAM01	82.6	78.6	4.9	76	8	acrylamide
CROTAM	81.4	77.2	5.3	83	–2	trans 2–butenoic acid amide
DIACHZ	104.1	98.5	5.3	96.5	7.3	1,2–diacetylhydrazine
DIKPIP03	106.6	123.8	–16.1	115.3	–8.2	2,5–piperazinedione
DIXTAF01	88	82.3	6.5	90.9	–3.3	2,2–dimethylpropanamide
FEPGEM	75	75.6	–0.7	87.8	–17	methyl carbamate
FORMAM02	72	66.2	8.2	66.3	8	formamide
GLUTIM	94	88	6.3	102.8	–9.3	glutarimide
IBURAM	86	79.1	8	81.1	5.7	2–methylpropanamide
KIKREC	101	108.2	–7.1	112.9	–11.7	N–propylurea
MALOAM02	126	129.1	–2.4	143.5	–13.9	malonamide
MEUREA01	97.4	95.2	2.3	94.5	3	N–methylurea
NIJHUJ04	89	80.5	9.6	86.8	2.5	1,3–dimethylurea
PYRZIN23	89.3	82.6	7.5	94	–5.3	pyrazine carboxamide
QQQGEM01	103	103.5	–0.4	119.8	–16.2	acetylurea
SUCCIN09	86.2	82.5	4.4	92.3	–7	succinimide
TFACAM	79	74.6	5.6	72.2	8.6	triFluoroacetamide
UREAXX25	97.6	94.2	3.5	102.2	–4.6	urea
WIFKEB02	95	91.2	4.1	90.3	5	1,1–dimethylurea
YAQLAE	97	98.2	–1.2	104	–7.2	N–ethylurea
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
YAQLEI	104.4	109.5	–4.8	118.2	–13.1	N–butylurea

ZZZKDQ01	85.3	87.8	–3	87.4	–2.5	butyramide
ZZZKJQ01	90	94.5	–4.9	98.7	–9.7	pentanamide
BZAMID12	100.2	93.6	6.7	99.2	1	benzamide
BZOXZO	98	101.6	–3.6	90.6	7.6	2–benzoxazolinone
CAPLAC	85.2	82.8	2.9	81.2	4.8	epsilon–caprolactam
EHOWIH	115	104.2	9.4	106.5	7.4	4–pyridinecarboxamide
NICOAM06	120	104.1	13.2	100.5	16.2	3–pyridinecarboxamide
PICAMD06	93.4	91	2.6	99.8	–6.8	2–pyridinecarboxamide
ACANIL06	87	98.2	–12.9	109.9	–26.4	acetanilide
HQOXAL01	120.9	104.4	13.6	95.2	21.2	2–hydroxyquinoxaline
PHALIM04	106	95.5	9.9	92.5	12.8	phthalimide
PHUREA02	138.2	121	12.4	128.9	6.7	monophenylurea
WIGYIV	107	100.4	6.2	91.1	14.8	1–(2H)–phthalazinone
REZRIY	97.6	97	0.6	106.8	–9.5	N– 2–methylphenyl acetamide
BRANIL	100	91.3	8.7	95.6	4.4	2,4,6–tribromoaniline
BRNIBZ	87	86.1	1.1	75.2	13.5	3–bromo–1–nitrobenzene
PBRANL01	79	73.3	7.2	74.7	5.5	4–bromoaniline
ULEBOD	87	87.1	–0.1	78.6	9.6	4–bromo–1–nitrobenzene
VOQYUW	82	75.8	7.6	69.7	15	2,5–dibromopyridine
YAQZUM	85	87.7	–3.2	75.6	11.1	2–bromo–1–nitrobenzene
BRBZAC01	109	110.7	–1.6	99.8	8.4	2–bromobenzoic acid
BRBZAP01	107	106.5	0.5	94.8	11.4	4–bromobenzoic acid
CAJWEQ01	88	82.5	6.2	82.5	6.3	2,4–dibromoaniline
QQQFDS02	102	104	–2	109.6	–7.5	9–bromoanthracene
FIZZOD	95	94	1.1	93.1	2.1	5–methyltetrazole
FULPIM	88.4	77.3	12.5	84.8	4.1	2–methylimidazole
IMAZOL13	83	71.8	13.5	70.5	15.1	imidazole
ITIZOA	72.1	74.5	–3.3	69.4	3.8	piperazine
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
TETZOL02	89	85.1	4.4	78.7	11.6	tetrazole
TRAZOL04	82	76	7.4	77.2	5.9	1,2,4–triazole
BZDMAZ04	100	96.4	3.6	97.4	2.6	benzimidazole
ZBCNON	58	65.8	–13.4	61.3	–5.8	3–azabicyclo 3.2.2nonane
CRBZOL03	101	99.8	1.2	104.2	–3.1	carbazole
KEMDOW	186	186	0	208.3	–12	guanine
DMANAP10	94.7	92	2.9	102.8	–8.5	1,8–N,N,N'N'–tetramethyldiaminonaphthalene
VUFZUR01	119.2	119.8	–0.4	131.7	–10.4	4–(N,N–dimethylamino azobenzene
BOTYIT	77	75.2	2.3	79.6	–3.4	2,4–dichloropyrimidine
DCPYAZ01	70	67.1	4.2	71.6	–2.2	2,6–dichloropyrazine
HAMGOT	89.4	88.2	1.4	95.1	–6.4	1,2,4–triazolo 1,5–apyrimidine
TELPOP	87	79.3	8.9	68.1	21.8	1–methyltetrazole
TRIZIN01	57	59.7	–4.6	65.3	–14.5	1,3,5–triazine
HXMTAM23	80	89.5	–11.9	71.5	10.6	1,3,5,7–tetraazatricyclo 3.3.1.13,7decane
ZZZIVG02	61.3	59.4	3	64.9	–5.9	4–methylpyridine

ZZZKAO01	61	59.1	3.1	64.7	–5.9	3–methylpyridine
DAZNAP	82	84.2	–2.6	86.4	–5.3	phthalazine
HEYJOK01	68	76.7	–12.8	74.4	–9.3	quinoxaline 1,4
MPYRAZ02	95	78.1	17.8	103.6	–9.1	tetramethylpyrazine
BIPYRL04	80	87.2	–9	97.2	–21.5	2,2 –bipyridine
CHLQUI10	84	86.3	–2.8	95.8	–14.1	2–chloroquinoline
CLQUIN	81	82.3	–1.6	84.2	–4	6–chloroquinoline
EYIRIN	102	104.7	–2.7	102.8	–0.8	1–benzylimidazole
KEYNOR	87.7	84.6	3.5	103.3	–17.8	2,3–dimethylquinoxaline
PHENAZ11	96	94.3	1.8	101.8	–6.1	phenazine
PILFOG	85	85.8	–1	94.9	–11.7	2,6–dimethylquinoline
NAMKAN01	100	102.5	–2.5	119.5	–19.5	4,4' –dimethyl–2–2'bipyridyl
CLBENQ	68.6	74.2	–8.3	82.3	–20	chlorobenzoquinone
DMEOXA06	75.3	81.4	–8.1	81	–7.6	dimethyl oxalate
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
ETHCAR	77	71.5	7.2	66.3	13.9	ethylene carbonate
LIJFUG	86	86.1	–0.2	102.6	–19.3	glutaric anhydride
MLEICA01	86.4	69.7	19.3	88.6	–2.5	maleic anhydride
NIKVUZ	69	57.1	17.3	80.9	–17.2	cyclobutane–1,2–dione
PTOXEC	88	91.3	–3.7	90.6	–3	1,3,5,7,9–pentoxecane
TOXOCN	80	80.9	–1.1	97.4	–21.7	1,3,5,7–tetroxane
TROXAN	56	63.3	–12.9	70.9	–26.5	1,3,5–trioxane
BNZQUI03	68.8	62.8	8.6	68	1.2	1,4–benzoquinone
CYHEXO01	84	78.2	6.9	95.5	–13.6	1,4–cyclohexanedione
GOCWEA	82	91.7	–11.8	80.4	2	trans–1,3,5,7–tetraoxadecalin
POKKAB	95	99.1	–4.3	109.6	–15.4	cis–1,3,5,7–tetraoxadecalin
ZZZDRQ01	85	91.4	–7.5	91.9	–8.2	dimethyl fumarate
BZCBUO	90.3	83.5	7.5	91.1	–0.9	benzocyclobutenedione
DMKETD02	71	69.1	2.7	82.1	–15.7	2,2,4,4–tetramethyl–1,3–cyclobutanedione
MOXBEN01	84	79.1	5.8	85.1	–1.3	1,4–dimethoxybenzene
PHTHAO	88.6	89.8	–1.3	95.5	–7.8	phthalic anhydride
COUMAR02	92.2	87.9	4.7	94.2	–2.1	coumarin
DMTPAL	105.1	110.3	–5	110.2	–4.9	dimethylthyl terephthalate
INDDON	97	84.8	12.6	92.6	4.5	1,3–indandione
NAPHQU01	91	88.9	2.3	96.2	–5.7	1,4–naphthoquinone
NBORAN02	97	96.7	0.3	103.6	–6.8	endo–5–norbornene–2,3–dicarboxylic anhydride
PYMDAN	122	115.9	5	149.5	–22.6	1,2,4,5–benzenetetracarboxylic acid anhydride
TMOXBZ10	100	89.2	10.8	93.4	6.6	1,3,5–trimethoxybenzene
BPHENO10	93	92.4	0.7	96	–3.2	benzophenone
BZDIOX01	92	92.9	–0.9	99.3	–7.8	dibenzo b,e 1,4 dioxin
CONYAH	93.1	95.2	–2.2	100	–7.4	xanthene
DBZFUR02	84	88.7	–5.5	90	–7.1	dibenzofuran
PARPEE	95	97.7	–2.8	104.7	–10.3	alpha naphthyl acetate

PHBENZ01	98	103.7	–5.8	107.7	–9.9	phenyl benzoate
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
RAFFIO01	82	86.2	–5.2	92.2	–12.4	diphenyl ether
ANTQUO08	111	113.1	–1.9	113.2	–2	9,10–anthraquinone
SAZQIT	101	103.1	–2.1	107.2	–6.2	2–fluorenecarboxaldehyde
HEGSAN01	117	113.3	3.1	92	21.4	1,4–dimethylcubane dicarboxylate
DBEZLM01	115	109	5.2	130.1	–13.1	dibenzoylmethane
ANTHAL	101	104	–3.1	112.1	–11.1	9–anthraldehyde
AHCHEX01	94.2	96.9	–2.9	90.6	3.9	alfa–hexachlorocyclohexane
HCCYHB	105.2	108.4	–3	105.8	–0.5	beta–hexachlorocyclohexane
DCLBEN03	65	68.7	–5.7	71.3	–9.6	1,4–dichlorobenzene
HCLBNZ14	97	97.3	–0.3	93.6	3.5	hexachlorobenzene
PNCLBZ	87	86.1	1.1	85.7	1.5	pentachlorobenzene
TCHLBZ03	72.9	70.9	2.8	77.4	–6.1	1,3,5–trichlorobenzene
DCLBIP	96	92.4	3.8	89.2	7.1	2,2' –dichlorobiphenyl
DCLBPH	150	140.1	6.6	143.1	4.6	decachlorobiphenyl fus+vap
FUHDAN01	123.9	121.5	2	125.7	–1.4	3,3',4,4'–tetrachlorobiphenyl
HCLBPH	102.7	107.5	–4.7	110.6	–7.6	2,2',4,4',6,6'–hexachlorobiphenyl
TCBZFU	124.5	121.2	2.6	122.5	1.6	2,3,7,8–tetrachlorodibenzofuran
TEKQIJ	100.6	113.2	–12.5	113.1	–12.4	2,2',5,5'–tetrachlorobiphenyl
DCLANT10	114	109.7	3.8	121	–6.2	9,10–dichloroanthracene
CLBENQ	68.6	74.2	–8.3	82.3	–20	chlorobenzoquinone
DCLBQN01	70	72.3	–3.3	95.7	–36.8	2,6–dichloro–1,4–benzoquinone
BIMVEZ	100	99.3	0.7	98.2	1.8	2–chlorobenzophenone
DCBDOX10	109.7	109.7	0	113.8	–3.7	2,8–dichlorodibenzo b,e 1,4 dioxin
DCBZDX20	111.2	119.6	–7.6	124.7	–12.1	2,7–dichlorodibenzo b,e 1,4 dioxin
FELSEU	112.9	124.7	–10.5	130.9	–15.9	1,2,3,4–tetrachlorodibenzo b,e 1,4 dioxin
OCDBDO10	150.7	160.7	–6.7	153.1	–1.6	octachlorodibenzo b,e 1,4 dioxin
SESHED	98	104.3	–6.4	108	–10.2	2–chlorodibenzo b,e 1,4 dioxin
BISJIW	70.6	65.6	7.2	68.4	3.2	fumaronitrile
CAACTY	41.2	30	27.3	30.2	26.7	cyanoacetylene
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
CYAPYR	75	68	9.4	67.9	9.5	4–cyanopyridine
CYNGEN	31.2	35.8	–14.6	49.8	–59.4	cyanogen
DCYANM	43.4	47.3	–8.8	63.3	–45.7	dicyanoacetylene
MALONT	79	61.4	22.3	80.7	–2.1	malononitrile
MUBZOY	71	74.5	–4.9	78.2	–10.1	2–cyanopyridine
MUBZUE	72	70.6	2	74.9	–4	3–cyanopyridine
QOPBED	70	72.8	–4	97.4	–39.1	succinonitrile
TCYETY11	83.5	78.6	5.8	142.9	–71.2	tetracyanoethylene
TCYMET	61	66.2	–8.6	134.7	–120.9	tetracyanomethane
BISJAO02	81	83.6	–3.2	98.2	–21.2	tetramethylsuccinonitrile
OBIZEE	90	87.9	2.4	94.3	–4.8	1,3–dicyanobenzene
TEPNIT11	90	89.6	0.4	94.8	–5.4	1,4–dicyanobenzene

YUYPUD02	87	85.2	2	95.9	–10.3	1,2–dicyanobenzene
JIBDON	84	76.3	9.2	84.2	–0.3	2,6–dimethylbenzonitrile
SUZXOB	94	95.5	–1.6	104.3	–10.9	2–cyanoquinoline
TCYQME03	120.6	115	4.7	148.6	–23.2	7,7,8,8–tetracyanoquinodimethane
XOGJAG	53.6	63.4	–18.3	57.9	–8	trifluoromethylbenzene
PUGPIQ	95.3	92.1	3.4	91.2	4.4	2,2' –difluorobiphenyl
ZZZAOS02	95	93.5	1.7	90.9	4.4	4,4' –difluorobiphenyl
DUCKOB03	32.2	32.6	–1.4	39.6	–22.9	butane
JAYDUI	24.8	26.9	–8.4	35.5	–43	propane
PENTAN01	38.9	41.9	–7.6	50.8	–30.6	pentane
QQQCIS01	25.7	27	–4.8	30.3	–17.7	cyclopropane
ZZZVYE01	39.5	41.7	–5.6	45.9	–16.1	cyclopentane
ZZZWEO02	32.9	33.9	–3	35.5	–7.9	cyclobutane
BENZEN18	44.6	44.9	–0.5	48.4	–8.4	benzene
HEXANE01	48.6	50.6	–4.1	59.7	–22.8	hexane
HEPTAN02	55.7	57.4	–3	66.8	–20	heptane
ZZZITY02	59.4	64	–7.9	71.8	–20.9	1,4–dimethylbenzene
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
BULVAL03	72	70.2	2.4	72.4	–0.6	bullvalene
DURENE	73	68.7	5.9	80.4	–10.1	1,2,4,5–tetramethylbenzene
NAPHTA10	73	70	4.2	77.8	–6.6	naphthalene
BIPHEN04	82	84.5	–3.1	89.5	–9.1	biphenyl
DMNPTL02	83	82.9	0.2	93.2	–12.2	2,6–dimethylnaphthalene
FLUREN01	85	85	0	87.8	–3.3	fluorene
ZZZMKS01	86	89.1	–3.6	93.8	–9.1	diphenylmethane
ANTCEN14	97	95	2.1	107.2	–10.4	anthracene
PHENAN08	92	89.6	2.6	100	–8.7	phenanthrene
COPMUR	75	76	–1.3	88.6	–18.2	pentamethylbenzene
HMBENZ17	84	79.4	5.5	92.1	–9.6	hexamethylbenzene
BISDOY	83.3	91.3	–9.6	94.7	–13.7	9–methylfluorene
DITBOX01	93	93	0	94.3	–1.4	9,10–dihydroanthracene
MANTHR14	101	94.3	6.6	103.6	–2.6	9–methylanthracene
PYRENE02	101	95.2	5.8	104.2	–3.2	pyrene
TOKKIN	91.3	91.5	–0.3	91.9	–0.7	1–methylfluorene
BZPHAN01	106	110.4	–4.1	122.6	–15.6	benzo c phenanthrene
CLNIBZ01	82	79.6	2.9	75.6	7.8	1–chloro–3–nitrobenzene
CLNOBE02	103	119.3	–15.9	119.3	–15.8	1–chloro–2,4,6–trinitrobenzene
FINBIP	72	76.6	–6.3	73.1	–1.5	1,1,1–trinitroethane
SETVIX	81	79.8	1.5	74.6	7.8	1–chloro–2–nitrobenzene
BECJEY	90	100.1	–11.2	110.4	–22.6	2,3–dinitro–2,3–dimethylbutane
DNBENZ15	85	95.1	–11.9	87.1	–2.4	1,3–dinitrobenzene
DNITBZ11	95	101.8	–7.2	90	5.3	1,4–dinitrobenzene
NITOLU01	77	77.8	–1	81.4	–5.7	4–nitrotoluene
UCOVAL	96	95.2	0.8	88.9	7.4	1– chloromethyl –2–nitrobenzene

ZZZFYW02	93	101.1	–8.8	93.9	–1	1,2–dinitrobenzene
ZZZQSC02	99	102.4	–3.4	93	6.1	2,6–dinitrotoluene
TNPHNT	121.8	121.9	–0.1	131.7	–8.1	2,4,6–trinitrophenetole
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
NTRANT01	114.6	112.4	2	118.1	–3	9–nitroanthracene
BDTOLE11	94.9	100.7	–6.1	99.2	–4.5	tetrathiafulvene
BETHAZ01	71	82	–15.5	114.5	–61.3	2,1,3–benzothiadiazole
DITHAN03	71	77.4	–9	64.2	9.6	1,4–dithiane
DMSULO04	77	87.5	–13.6	84.3	–9.5	dimethyl sulfone
DTOLTO	82	81.5	0.6	78.1	4.8	1,3–dithiolan–2–thione
IXANOK	80	79.3	0.9	80.8	–1	1,3–dithiolan–2–one
OFIZEK	84	87	–3.6	81.4	3	tetramethylthiourea
OWEKEH	73	76.8	–5.2	80.3	–10	tetrahydro–4H–thiopyran–4–one
PUVVUZ	89.2	94.1	–5.5	85.3	4.4	1,3–dithian–2–thione
THIOUR16	108.6	84.4	22.3	69.8	35.7	thiourea
TPENAC02	97.4	95.4	2.1	91.8	5.8	2–thiophene carboxylic acid
TRITAN10	94	86.6	7.9	72.3	23.2	1,3,5–trithiane
YIFZAP	115	113.7	1.1	104.6	9	benzenesulfonamide
DTENYL02	85.6	88.5	–3.4	108.6	–26.8	2,2 –bithiophene
MPSUFO01	92	96.5	–4.9	87	5.4	MEphenylsulfone
FABPON11	123	114.2	7.1	126.3	–2.7	5–phenyl–1,2–dithiole–3–thione
PRYLTS	96	111.6	–16.2	110.9	–15.5	p–tolyl propenylsulfone
DBZTHP	96	96.9	–0.9	103.8	–8.1	dibenzothiophene
DPSULO	106	112.2	–5.8	104.1	1.7	diphenyl sulfone
PHESAZ01	115	106.8	7.1	106.8	7.1	phenothiazine
THIANT03	100	107.6	–7.6	100.7	–0.6	thianthrene
TOXANT	101	100.8	0.2	102.7	–1.7	thioxanthene
MOYGUC01	62.2	77.6	–24.8	74.2	–19.3	thiocamphor
TUXFIC02	125	142.7	–14.1	140	–12	dibenzyl sulfone
AMIPYR	83	74.7	10	76.3	8.1	3–aminopyridine
AMMTAZ01	91.8	93.8	–2.2	97.9	–6.6	2–methyl–5–aminotetrazole
AMPYRD	78	71.6	8.3	83	–6.4	2–aminopyridine
AMPYRE01	88	83.8	4.8	90.1	–2.4	4–aminopyridine
CSD name	ΔH_s	E_{LJC}	D%	E_{CLP}	D%	compound name
CAGPUV01	85	84.8	0.2	79.5	6.5	3,4–dichloro–1–nitrobenzene
CARDOO	109	98.4	9.7	107.6	1.3	4,5–dichloro–2–nitroaniline
CLNOAN	109	101.2	7.2	109.6	–0.6	2,6–dichloro–4–nitroaniline
CUVJUY	101.9	99.3	2.6	102.5	–0.6	1,4–diNOpiperazine
DATNBZ01	145	135.2	6.7	171.3	–18.2	1,3–diamino–2,4,6–trinitrobenzene
DCHLAN01	83	79.8	3.9	87.7	–5.7	2,5–dichloroaniline
GETVEH	74	77.4	–4.7	79.4	–7.3	2,3,5–trichloropyridine
HIBWEU	83	81.8	1.5	82	1.2	3,5–dichloro–1–nitrobenzene
KOMYEQ01	80	82.6	–3.3	96.2	–20.2	N–methylsuccinimide
LETNAZ01	103	97.5	5.3	99.9	3	3,5–dimethyl–4–NOpyrazole

NANILI31	101	98.6	2.4	104.8	–3.8	4–nitroaniline
NICOAC02	115	102.2	11.1	92.4	19.7	3–pyridinecarboxylic
PICANO04	95.8	93.9	2	96.9	–1.1	pyridine–2–carboxylic acidNoxide
RAKSIG	151.7	147.8	2.6	142.6	6	6–mercaptopurine
UCECAG02	115	115.3	–0.3	118.9	–3.4	2–chloro–4,6–dinitroaniline
WEMDAT	82	74.1	9.7	81.2	0.9	2,3–dichloroaniline
WEMDEX	74	71.9	2.9	79.6	–7.5	2,6–dichloroaniline
WEMDIB	85	77.4	8.9	84.3	0.8	2,4–dichloroaniline
XAGWIM02	100.2	101.7	–1.4	99.1	1.2	pyrrole–2–carboxylic acid
YOVCAO	100	98.5	1.5	106.2	–6.2	2–chloro–5–nitroaniline
ZZZEKW02	87	82.4	5.3	77.5	11	2,5–dichloro–1–nitrobenzene
AMBACO08	110	96.4	12.3	100.4	8.8	2–aminobenzoic acid
BEOXAZ	65	75.2	–15.6	64.5	0.8	benzofurazan
BIPJUF	135	134.9	0.1	121.5	10	2,4–dinitrobenzoic acid
CLANIC06	86	73.1	15	80.8	6	4–chloroaniline
MEADEN05	124	127.8	–3	142.3	–14.7	9–methyladenine
NBZOAC12	120	118.8	1	110.9	7.6	4–nitrobenzoic acid
NBZOAO04	119	115.8	2.7	113.4	4.7	2–nitrobenzoic acid
PNBZNT	91	92.7	–1.9	90.8	0.2	4–nitrobenzonitrile
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
RAJGUG	89	70.6	20.7	69.8	21.5	2–methylpyridine Noxide
RICFEP01	81	78.6	3	86.4	–6.7	2–acetylpyrrole
TNIOAN02	125.2	129.1	–3.1	143.4	–14.5	2,4,6–trinitroaniline
AMACPH01	93.3	98.8	–5.9	113.3	–21.5	4–aminoacetophenone
AMBNAC12	116	116.2	–0.2	108.4	6.6	4–aminobenzoic acid
AMEBAC	107	103.9	2.9	116.6	–9	2–amino–3–methylbenzoic acid
ANISIC04	111	109.3	1.6	105.9	4.6	4–methoxybenzoic acid
DIMNAN01	102	105.9	–3.8	116.2	–13.9	N,N–dimethyl–4–nitroaniline
DMADEN11	117	109.7	6.3	119.4	–2	N,N–dimethyladenine
FUFBOX	107	108.8	–1.7	108.1	–1	2–methoxybenzoic acid
MBNZAM10	83.2	88.6	–6.4	89.1	–7	N–methylbenzamide
MNTDMA01	93	96.5	–3.8	98.3	–5.7	3–nitro–N,N–dimethylaniline
MODYAG01	138.2	122	11.7	134.9	2.4	4–aminophthalimide
DMOXBA01	122	128.8	–5.6	133.5	–9.4	2,6–dimethoxybenzoic acid
DMXBZA01	130	117	10	117.6	9.6	3,4–dimethoxybenzoic acid
HEKMOZ	127	123	3.1	121.3	4.5	3,5–dimethoxybenzoic acid
ISUQUI	123	126.2	–2.6	120.4	2.1	2,4–dimethoxybenzoic acid
ISURAP	116	109.9	5.3	119.5	–3	2,5–dimethoxybenzoic acid
NONMEI	93	83.4	10.4	96.6	–3.8	8–aminoquinoline
ODOTOQ	93	84.4	9.2	86.8	6.6	N,N–dimethylbenzamide
PICGAJ	109	109.2	–0.2	126.9	–16.4	3–amino–1–phenyl–but–2–enone
SECQEY	104	96.3	7.4	101.1	2.7	3–aminoquinoline
UPAJIF	107	104.5	2.3	102.1	4.6	8–nitroquinoline
VAKJUM	124	105	15.3	109.1	12	2,3–dimethylquinoxaline 1,4dioxide

ZZZFLM01	129	117.5	8.9	116.6	9.6	trans–2–methoxycinnamic
ZZZPRC03	106	88.3	16.7	100.6	5.1	1–methyl–1H–indole–2,3–dione
CINMAC	107	101.8	4.9	96.4	9.9	trans cinnamic acid
MXCINN02	134	117.2	12.5	113.3	15.4	trans–4–methoxycinnamic
OVERAT01	117	121.7	–4	120.2	–2.8	2,3–dimethoxybenzoic acid
CSD name	ΔH_s	E_{LIC}	D%	E_{CLP}	D%	compound name
PEXBZA	123	117.5	4.5	112.9	8.2	4–ethoxybenzoic acid
ZZZNRU02	124	118.6	4.4	116.2	6.3	trans–3–methoxycinnamic
HIBXOF	135	126.6	6.2	140	–3.7	acridone
DMPIPA	80	80.9	–1.2	91.3	–14.2	2–methyl–2–piperidinopropionitrile
EACDRO01	117	117	0	133	–13.7	10–ehylacridin–9(10H)–one
NMACRO11	105	118.4	–12.8	126.5	–20.5	10–methylacridin–9 10H –one
FEXBOZ	87	89.7	–3.1	105.6	–21.4	benzylidene t–Bu amine Noxide