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Table SI1. Investigated structures, literature experimental melting points, literature sources, and some experimental details taken from Beilstein database (ref. S0).

N-substituent	Other substituents	ID	Melting point (K)	Notes: crystallized from; other properties.	ref.
decyl	3-pentyl	1	303		S1
11-propionyloxyundecyl		2	308		S2
benzyl	4-dibenzyl, 3-ethoxycarbonyl	3	308		S3
octyl	4-propyl	4	309-311		S1
tetradecyl	4-hexyl	5	309-311	diethyl ether	S1
tetradecyl	3-pentyl	6	311-313	acetone, diethyl ether	S1
decyl	4-ethoxycarbonyl	7	313-314		S4
dodecyl	4-propyl	8	313-315	diethyl ether	S1
undecyl		9	314.4-315.4	ethanol, ethyl acetate	S5
octyl	4-ethyl	10	314-317	acetone	S1
dodecyl	4-ethyl	11	316-317	acetone, diethyl ether	S1
decyl		12	316-319		S6
			309.5-310.8	ethanol, ethyl acetate	S5
dodecyl		13	362-363	ethanol, diethyl ether	S7
			347-348	butan-2-one; with 1 mol H_2O	S8
			320-320.4	ethanol, ethyl acetate	S5
			317.5-318.5		S9
hexyl	2-(2-methyloctyl)	14	319-321	diethyl ether	S1
ethoxycarbonylmethyl	5-butyl; 2-methyl	15	324		S3
2,5-dimethoxyphenethyl		16	326-327.5	ethanol	S10
tridecyl		17	327-328	benzene, petroleum ether	S11
			322-323	ethanol, ethyl acetate	S5
4-fluoro-benzyl		18	330-331	acetone, ethanol	S12
tetradecyl		19	331.5-332.5	acetone	S5
			327.5-328.5		S9
butyl	4-ethoxycarbonyl	20	333		S4
2-methylpropyl		21	336-338	ethanol, diethyl ether; with 1 mol H_2O	S13
methyl	3-(3-hydroxypropyl)	22	337		S14
benzyl	3-methyl	23	337-338	ethanol, chloroform	S15
butyl	2-benzylsulfanyl	24	338		S16
2-cyclohexyl-2-oxo-ethyl		25	342		S3
methylpropyl		26	342-343	ethanol, diethyl ether; with 1 mol H_2O	S13
2-pyridinyl		27	343-343.8	ethanol, diethyl ether	S17
2-(ethoxycarbonyl)ethyl		28	343-345	acetone	S18

N-substituent	Other substituents	ID	Melting point (K)	Notes: crystallized from; other properties.	ref.
1-(ethoxycarbonyl)-propyl		29	346		S19
propyl		30	348-349	ethanol, diethyl ether	S13
ethyl	3-diethylcarbamoyl	31	350	ethanol, diethyl ether	S20
2-phenoxyethyl		32	353-356		S21
			351		S22
methyl	2,4,6-trimethyl	33	351	ethanol, diethyl ether; with 2 mol H_2O	S23
methyl	4-(3-hydroxypropyl)	34	351-353	ethanol, acetone	S24
ethyl	2,6-dimethyl	35	353	hygroscopic	S25
methyl	3-pyridinyl	36	353		S3
Isopropyloxycarbonyl-methyl		37	363-364	ethanol, acetone	S26
			352-354		S27
morpholinomethyl	4-methyl	38	355-356	ethanol, ethyl acetate	S28
methyl	4-benzyl	39	357-360		S29
2-fluoroethyl	3-ethoxycarbonyl	40	359-361	hygroscopic	S30
phenethyl	4-methyl	41	361.8-364	ethanol, diethyl ether	S31
butyl	3-carboxy	42	364	with 1 mol H_2O	S32
allyl	3-diethylcarbamoyl	43	365	with 1 mol H_2O, hygroscopic	S33
bis(ethoxycarbonyl)-methyl		44	366-367		S34
			343-344		S35
4-acetoxybutyl	3-hydroxy	45	367-369	ethanol, ethyl acetate	S36
benzyloxy		46	367-368		S37
allyl		47	368-369		S38
			365-367	ethanol, diethyl ether; hygroscopic	S39
methyl	3-ethoxycarbonyl	48	368-370		S40
			323.5-324	hygroscopic	S41
2-hydroxyethyl	3-methyl	49	368-372	ethanol, acetone; with 0.5 mol H_2O	S42
ethyl	2-methyl	50	370	ethanol	S43
			338	acetone	S44
isopropyl		51	370		S45
butyl		52	370-371		S46
ethyl	4-(4-pyridyl)	53	371	acetone, diethyl ether	S47
			338-343		S48
allyl	3-hydroxy	54	370-372	ethanol, diethyl ether	S36
benzyl		55	383	acetonitrile	S49
			371-373	ethanol, diethyl ether; with 2 mol H_2O, hygroscopic	S50
methyl	4-(2-ethoxycarbon-ylethyl)	56	372-373	diethyl ether	S51
ethyl	3-acetyl	57	373		S52
allyl	3-formyl	58	373		S53

N-substituent	Other substituents	ID	Melting point (K)	Notes: crystallized from; other properties.	ref.
acetonyl	2,6-dimethyl	59	377		S54
ethyl	3-hydroxy	60	378-380		S55
			372-375	ethanol	S36
ethoxy	4-methoxy	61	381-382	acetone	S56
Propyloxycarbonyl-methyl		62	383		S27
			382.5-384		S57
allyl	2-hydroxymethyl	63	383		S58
2-hydroxyethyl		64	383	ethanol	S59
			381-383		S60
			372-376	ethanol	S61
			370-375	ethanol, methan-ol, diethyl ether; hygroscopic	S62
allyl	4-hydroxymethyl	65	384		S58
5-hexynyl		66	386-388	acetonitrile	S63
2-cyanoethyl	3-methyl	67	388-390		S64
pyridinyl		68	456-458	ethanol, ethyl acetate	S65
			390-392	ethanol	S66
isopropyl	4-hydroxymethyl	69	392		S58
3-chloropropyl		70	393	acetone	S67
ethyl		71	393-394	ethanol, diethyl ether	S68
			391-392		S69
allyl	4-cyano	72	393-395	methanol, diethyl ether	S70
ethyl	4-methyl	73	394	ethanol	S71
isopropyl	2-hydroxymethyl	74	395		S58
2-hydroxyethyl	3-hydroxy	75	395-396	ethanol, heptane	S36
2-hydroxyethyl	3,4-dimethyl	76	398-401		S72
3,3-dimethylallyl	4-methyl	77	399-402		S73
1-methyl-2-oxopropyl	2-methyl	78	406	acetone	S74
2-cyanoethyl	3,4-dimethyl	79	405-407		S64
ethoxycarbonylmethyl		80	409-411		S57
			408-409	acetone	S35
			407		S76
			407-409	methanol, toluene	S75
			405		S18
			406-408		S77
			393-396		S78
3-bromopropyl	4-methyl	81	412-413	ethanol, diethyl ether	S79
			314	ethanol, diethyl ether, dichloromethane	S80
(Z)-3-methylpent-2-en-4-inyl		82	412-413	acetonitrile, diethyl ether	S81
methyl	3-methoxycarbonyl	83	413-415	hygroscopic	S41
			344		S82
2-cyanoethyl	3-amino	84	414-416	hygroscopic	S64
1-methyl-2-oxopropyl		85	417		S84
			416-417	ethanol, dietyl ether	S83
cyanomethyl	3,5-dimethyl	86	416-418		S85

N-substituent	Other substituents	ID	Melting point (K)	Notes: crystallized from; other properties.	ref.
methyl	4-methyl-3-hydroxy	87	418.5-419		S86
2-cyanoethyl	4-methyl	88	419-421		S64
2-cyanoethyl		89	421-423		S64
methyl		90	423		S45
			408,5	methanol; hygroscopic	S87
methyl	3-hydroxy	91	426-427	ethanol	S88
			421-423		S89
vinyl		92	427-428	ethanol, diethyl ether	S68
			421-423	with 1 mol H_2O	S42
phenyl		93	428	hygroscopic	S90
(E)-3-hydroxyprop-1-en-1-yl		94	429-430	acetonitrile	S91
2-carboxyallyl		95	429.5		S3
cyclohex-2-enyl		96	432-433		S92
2-cyanoethyl	3,5-dimethyl	97	433-434		S64
3-carboxypropyl		98	435-437	acetonitrile, methanol	S93
			434		S94
methyl	4-methoxycarbonyl	99	436-438	chloroform	S95
ethyl	4-cyano	100	438-439		S96
cyanomethyl		101	439-441		S97
			439-440		S78
			433		S98
			434	ethanol	S99
methyl	2-hydroxymethyl	102	439-442	ethanol	S100
vinyl	4-methyl	103	441-443	ethanol, acetone; with 1 mol H_2O	S42
isopropyl	4-methoxy	104	442-443		S96
methyl	4-methyl	105	445-447	acetonitrile; hygroscopic	S101
methoxycarbonylmethyl		106	447-448	propan-2-ol, butan-2-one	S27
			443-446		S78
			437-438		S57
methyl	3-carbamoyl	107	448	ethanol	S102
			445		S32
ethyl	4-dimethylamino	108	449	ethanol, ethyl acetate	S65
prop-2-ynyl	4-methyl	109	450-452	ethanol, diethyl ether	S103
cyanomethyl	4-methyl	110	451-453		S97
2-fluoroethyl		111	453	hygroscopic	S30
methyl	4-acetyl	112	456-457	ethanol	S104
			457-457	butan-1-olo	S105
allyl	4-(hydroxyimino-methyl)	113	456-460	ethanol	S106
Hydrazinocarbonyl-methyl		114	458-459	ethanol	S107
2-oxopropyl		115	459-461		S77
			457		S57
			458	ethanol	S108
ethyl	4-carbamoyl	116	461		S4
(E)-2-carboxy-1-ethenyl		117	461-462	propan-2-olo	S91

N-substituent	Other substituents	ID	Melting point (K)	Notes: crystallized from; other properties.	ref.
2-propionamido		118	462-463		S109
(E)-2-carboxy-1-ethenyl	3-methyl	119	463-464	ethanol	S91
allyl	2-(hydroxyimino-methyl)	120	465-466	ethanol	S110
2-oxopropyl	2-methyl	121	469	ethanol	S111
			469	ethanol	S112
			468-470		S113
			463-465		S114
2-hydroxyethyl	2-(hydroxyimino-methyl)	122	470-473	ethanol	S106
cyanomethyl	2,4-dimethyl	123	471-473		S115
carboxymethyl		124	471-473	acetonitrile, methanol	S93
			456-460	ethanol	S116
			471-473	ethanol	S117
2-carbamoylethyl		125	476.5-477.5		S57
carbamoylmethyl		126	473		S109
			473	ethanol, water	S118

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Table SI2a. Cross validation. Training set B+C (84 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
2	308.15	317.55	9.40	4.73
3	308.15	306.28	-1.87	11.85
5	310.15	307.02	-3.13	10.10
6	312.15	305.78	-6.37	10.99
8	314.15	309.54	-4.61	8.94
9	315.05	318.62	3.57	7.14
11	316.65	322.61	5.97	10.57
12	317.65	317.79	0.14	8.25
14	320.15	319.46	-0.69	11.76
15	324.15	322.88	-1.27	9.26
17	327.65	318.51	-9.14	7.09
18	330.65	342.62	11.97	12.77
20	333.15	348.88	15.73	12.13
21	337.15	350.04	12.89	12.88
23	337.65	336.83	-0.82	10.34
24	338.15	342.39	4.24	8.24
26	342.65	353.17	10.52	10.05
27	343.55	366.09	22.54	12.08
29	346.15	355.27	9.12	12.09
30	348.65	369.66	21.01	10.69
32	351.15	352.02	0.87	10.53
33	351.65	364.89	13.24	7.86
35	353.15	349.91	-3.24	9.72
36	353.15	358.64	5.49	8.99
38	355.65	374.20	18.55	14.63
39	358.65	369.41	10.76	9.26
41	363.05	360.71	-2.34	10.35
42	364.15	376.40	12.25	13.06
44	366.65	361.59	-5.06	14.54
45	368.15	372.96	4.81	10.53
47	368.65	381.97	13.32	11.74
48	369.15	378.50	9.35	7.83
50	370.15	386.47	16.32	14.49
51	370.15	372.40	2.25	9.66
53	371.15	369.19	-1.96	15.40
54	371.15	376.62	5.47	11.58
56	372.65	374.03	1.38	11.79
57	373.15	383.66	10.51	11.22
59	377.15	373.25	-3.90	8.63
60	379.15	389.58	10.43	13.22
62	383.15	367.53	-15.62	10.42
63	383.15	398.47	15.32	14.71
65	384.15	394.66	10.51	14.08

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
66	387.15	393.32	6.17	16.60
68	391.15	392.14	0.99	9.65
69	392.15	391.21	-0.94	13.44
71	393.65	391.57	-2.08	6.70
72	394.15	418.34	24.19	11.51
74	395.15	390.89	-4.26	9.04
75	395.65	403.75	8.10	10.96
77	400.65	394.25	-6.40	13.09
78	406.15	401.17	-4.98	11.53
80	410.15	391.15	-19.00	12.36
81	412.65	409.51	-3.14	13.26
83	414.15	398.95	-15.20	10.57
84	415.15	418.98	3.83	12.70
86	417.15	416.23	-0.92	8.07
87	418.95	418.86	-0.09	7.71
89	422.15	427.53	5.38	13.49
90	423.15	418.43	-4.72	9.05
92	427.65	421.96	-5.69	18.18
93	428.15	398.66	-29.49	18.02
95	429.65	432.30	2.65	10.83
96	432.65	422.88	-9.77	15.01
98	436.15	436.98	0.83	8.64
99	437.15	445.31	8.16	9.80
101	440.15	439.13	-1.02	12.27
102	440.65	433.65	-7.00	5.33
104	442.65	421.12	-21.53	17.10
105	446.15	439.09	-7.06	10.19
107	448.15	411.31	-36.84	10.99
108	449.15	446.12	-3.03	10.96
110	452.15	454.85	2.70	13.15
111	453.15	449.94	-3.21	10.79
113	458.15	426.05	-32.10	9.92
114	458.65	457.22	-1.43	10.13
116	461.15	450.94	-10.21	11.74
117	461.65	463.73	2.08	11.68
119	463.65	459.22	-4.43	12.00
120	465.65	440.76	-24.89	13.30
122	471.65	469.35	-2.30	11.46
123	472.15	462.63	-9.52	11.25
125	472.15	459.17	-12.98	6.69
126	473.15	464.52	-8.63	11.54

Table SI2b. Cross validation. Test set A (42 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
1	303.15	305.74	2.59	10.90
4	310.15	311.20	1.05	9.41
7	313.65	325.12	11.47	15.35
10	315.65	325.96	10.31	11.34
13	318.15	317.86	-0.29	8.68
16	326.95	360.48	33.53	34.16
19	332.15	318.18	-13.97	8.87
22	337.15	388.72	51.57	17.24
25	342.15	401.89	59.74	28.42
28	344.15	369.72	25.57	16.38
31	350.15	421.37	71.22	27.21
34	352.15	407.53	55.38	26.33
37	353.15	370.28	17.13	18.15
40	360.15	407.69	47.54	26.39
43	365.15	372.66	7.51	23.40
46	368.15	367.96	-0.19	20.51
49	370.15	401.22	31.07	17.38
52	370.65	355.47	-15.18	14.92
55	372.15	365.15	-7.00	21.04
58	373.15	385.27	12.12	16.97
61	381.65	431.58	49.93	23.37
64	383.15	428.17	45.02	22.76
67	389.15	402.83	13.68	16.05
70	393.15	420.37	27.23	22.20
73	394.15	419.81	25.65	19.97
76	399.65	402.78	3.13	26.05
79	406.15	416.23	10.08	31.73
82	412.65	404.06	-8.59	32.52
85	417.15	389.89	-27.26	18.95
88	420.15	436.35	16.20	17.07
91	426.65	410.80	-15.85	15.01
94	429.65	434.86	5.21	33.84
97	433.65	400.21	-33.44	19.37
100	438.65	441.26	2.61	25.69
103	442.15	443.58	1.43	34.55
106	447.65	403.50	-44.15	18.66
109	451.15	431.38	-19.77	23.85
112	456.65	439.09	-17.56	10.19
115	460.15	409.78	-50.37	21.41
118	462.65	438.50	-24.15	23.92
121	469.15	408.73	-60.42	12.13
124	472.15	449.98	-22.17	17.99

Table SI3a. Cross validation. Training set A+C (84 molecules). Results averaged over 16 trials (threshold: 50 K).

name	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
1	303.15	300.29	-2.86	9.55
3	308.15	313.01	4.86	9.11
4	310.15	305.33	-4.82	7.68
6	312.15	306.36	-5.79	7.46
7	313.65	310.57	-3.08	6.68
9	315.05	324.57	9.52	13.46
10	315.65	311.08	-4.57	8.84
12	317.65	325.10	7.45	8.40
13	318.15	325.60	7.45	7.18
15	324.15	318.15	-6.00	11.49
16	326.95	344.50	17.55	17.43
18	330.65	344.41	13.76	9.28
19	332.15	327.06	-5.09	7.36
21	337.15	344.19	7.04	13.62
22	337.15	345.45	8.30	11.61
24	338.15	343.55	5.40	10.46
25	342.15	359.08	16.93	17.19
27	343.55	367.44	23.89	11.34
28	344.15	351.62	7.47	13.46
30	348.65	362.24	13.59	11.95
31	350.15	369.23	19.08	18.13
33	351.65	353.96	2.31	13.20
34	352.15	362.74	10.59	14.18
36	353.15	361.70	8.55	10.38
37	353.15	354.39	1.24	13.05
39	358.65	368.42	9.77	18.72
40	360.15	372.29	12.14	11.00
42	364.15	360.95	-3.20	12.92
43	365.15	364.51	-0.64	9.11
45	368.15	363.41	-4.74	13.98
46	368.15	371.68	3.53	13.03
48	369.15	362.30	-6.85	5.36
49	370.15	371.38	1.23	7.81
51	370.15	375.67	5.52	14.54
52	370.65	353.80	-16.85	12.35
54	371.15	374.04	2.89	7.56
55	372.15	374.47	2.32	18.49
57	373.15	373.98	0.83	8.37
58	373.15	370.09	-3.06	9.26
60	379.15	384.50	5.35	12.55
61	381.65	388.77	7.12	13.44
63	383.15	402.33	19.18	12.64
64	383.15	394.72	11.57	11.92

name	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
66	387.15	388.98	1.83	19.43
67	389.15	387.93	-1.22	11.20
69	392.15	379.50	-12.65	14.38
70	393.15	394.39	1.24	16.84
72	394.15	402.26	8.11	10.61
73	394.15	411.87	17.72	11.65
75	395.65	392.41	-3.24	8.58
76	399.65	398.71	-0.94	7.45
78	406.15	419.91	13.76	10.65
79	406.15	406.75	0.60	8.18
81	412.65	411.61	-1.04	11.03
82	412.65	417.94	5.29	15.62
84	415.15	409.63	-5.52	10.90
85	417.15	419.20	2.05	9.74
87	418.95	421.73	2.78	13.63
88	420.15	426.50	6.35	9.54
90	423.15	418.37	-4.78	12.45
91	426.65	412.24	-14.41	13.89
93	428.15	401.35	-26.80	14.26
94	429.65	427.70	-1.95	15.92
96	432.65	414.78	-17.87	14.78
97	433.65	433.85	0.20	5.91
99	437.15	433.59	-3.56	9.91
100	438.65	425.65	-13.00	13.37
102	440.65	433.77	-6.88	10.27
103	442.15	434.38	-7.77	14.95
105	446.15	439.39	-6.76	10.52
106	447.65	438.84	-8.81	9.76
108	449.15	427.47	-21.68	17.87
109	451.15	447.34	-3.81	11.36
111	453.15	434.51	-18.64	16.18
112	456.65	439.39	-17.26	10.52
114	458.65	459.71	1.06	8.93
115	460.15	449.21	-10.94	11.78
117	461.65	463.47	1.82	9.37
118	462.65	461.53	-1.12	6.93
120	465.65	444.05	-21.60	13.77
121	469.15	464.55	-4.59	12.80
123	472.15	468.25	-3.90	13.52
124	472.15	459.80	-12.35	6.96
126	473.15	464.59	-8.56	7.62

Table SI3b. Cross validation. Test set B (42 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
2	308.15	324.70	16.55	15.01
5	310.15	307.71	-2.44	28.33
8	314.15	309.82	-4.33	13.75
11	316.65	317.48	0.83	16.54
14	320.15	336.92	16.77	28.52
17	327.65	325.83	-1.82	13.67
20	333.15	338.01	4.86	22.07
23	337.65	344.08	6.43	38.01
26	342.65	347.12	4.47	18.45
29	346.15	380.33	34.18	36.95
32	351.15	358.96	7.81	33.02
35	353.15	333.02	-20.13	35.96
38	355.65	446.51	90.86	11.94
41	363.05	391.15	28.10	28.17
44	366.65	369.98	3.33	24.35
47	368.65	386.31	17.66	17.17
50	370.15	402.07	31.92	31.45
53	371.15	373.26	2.11	36.38
56	372.65	372.95	0.30	31.46
59	377.15	383.41	6.26	33.09
62	383.15	352.01	-31.14	16.74
65	384.15	377.39	-6.76	30.49
68	391.15	395.46	4.31	30.86
71	393.65	391.85	-1.80	18.46
74	395.15	382.84	-12.31	26.41
77	400.65	403.70	3.05	33.60
80	410.15	373.27	-36.88	18.34
83	414.15	390.37	-23.78	18.92
86	417.15	447.12	29.97	14.79
89	422.15	415.43	-6.72	21.01
92	427.65	406.37	-21.28	30.67
95	429.65	450.69	21.04	18.24
98	436.15	413.70	-22.45	29.87
101	440.15	441.15	1.00	20.85
104	442.65	405.80	-36.85	16.52
107	448.15	371.72	-76.43	14.37
110	452.15	449.90	-2.25	16.13
113	458.15	401.40	-56.75	15.80
116	461.15	420.63	-40.52	28.90
119	463.65	417.83	-45.82	21.03
122	471.65	432.70	-38.95	27.18
125	472.15	438.66	-33.49	20.91

Table SI4a. Cross validation. Training set A+B (84 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
1	303.15	298.56	-4.59	8.32
2	308.15	330.19	22.04	4.58
4	310.15	308.64	-1.51	7.62
5	310.15	306.51	-3.64	7.06
7	313.65	316.98	3.33	9.60
8	314.15	306.83	-7.32	7.64
10	315.65	315.33	-0.32	6.46
11	316.65	313.31	-3.34	6.89
13	318.15	330.21	12.06	4.56
14	320.15	323.57	3.42	8.04
16	326.95	339.79	12.84	10.22
17	327.65	330.08	2.43	4.66
19	332.15	330.16	-1.99	4.60
20	333.15	333.31	0.16	11.07
22	337.15	349.10	11.95	10.53
23	337.65	343.24	5.59	12.90
25	342.15	340.79	-1.36	11.90
26	342.65	351.53	8.88	10.24
28	344.15	365.87	21.72	10.95
29	346.15	359.58	13.43	13.31
31	350.15	365.46	15.31	16.61
32	351.15	346.46	-4.69	9.23
34	352.15	359.10	6.95	12.05
35	353.15	350.15	-3.00	13.19
37	353.15	367.65	14.50	17.28
38	355.65	374.84	19.19	18.76
40	360.15	353.01	-7.14	14.01
41	363.05	361.89	-1.16	12.04
43	365.15	366.11	0.96	10.40
44	366.65	360.90	-5.75	12.08
46	368.15	359.11	-9.04	16.01
47	368.65	390.63	21.99	13.80
49	370.15	379.82	9.67	12.92
50	370.15	390.85	20.70	8.21
52	370.65	360.21	-10.44	12.95
53	371.15	386.00	14.85	11.66
55	372.15	372.04	-0.11	14.00
56	372.65	363.43	-9.22	10.67
58	373.15	385.96	12.81	14.14
59	377.15	388.61	11.46	9.67
61	381.65	400.75	19.10	16.25
62	383.15	363.53	-19.62	12.79
64	383.15	407.47	24.32	13.37

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
65	384.15	398.11	13.96	8.35
67	389.15	396.66	7.51	10.17
68	391.15	398.07	6.92	14.44
70	393.15	381.06	-12.09	12.78
71	393.65	392.25	-1.40	13.26
73	394.15	400.12	5.97	14.04
74	395.15	397.72	2.57	10.97
76	399.65	401.51	1.86	11.58
77	400.65	398.29	-2.36	13.91
79	406.15	418.61	12.46	10.18
80	410.15	377.22	-32.93	11.08
82	412.65	430.84	18.19	15.14
83	414.15	413.38	-0.77	13.69
85	417.15	428.82	11.67	11.00
86	417.15	424.66	7.51	9.24
88	420.15	430.12	9.97	8.85
89	422.15	431.88	9.73	8.59
91	426.65	429.33	2.68	15.26
92	427.65	421.79	-5.86	11.64
94	429.65	425.66	-3.99	11.26
95	429.65	447.88	18.23	11.75
97	433.65	418.86	-14.79	10.07
98	436.15	426.67	-9.48	14.31
100	438.65	440.23	1.58	11.04
101	440.15	438.54	-1.61	11.20
103	442.15	434.48	-7.67	13.23
104	442.65	420.18	-22.47	13.67
106	447.65	439.09	-8.56	15.32
107	448.15	426.72	-21.43	13.27
109	451.15	447.03	-4.12	13.68
110	452.15	443.09	-9.06	8.48
112	456.65	440.16	-16.49	13.34
113	458.15	435.70	-22.45	13.84
115	460.15	442.94	-17.21	14.86
116	461.15	446.41	-14.74	11.17
118	462.65	452.17	-10.48	11.28
119	463.65	444.46	-19.19	15.29
121	469.15	444.91	-24.24	7.85
122	471.65	450.24	-21.41	12.37
124	472.15	456.05	-16.10	11.58
125	472.15	446.64	-25.51	12.78

Table SI4b. Cross validation. Test set C (42 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
3	308.15	317.57	9.42	24.22
6	312.15	298.07	-14.08	8.66
9	315.05	330.16	15.11	4.59
12	317.65	330.72	13.07	4.19
15	324.15	317.75	-6.40	15.05
18	330.65	379.68	49.03	24.25
21	337.15	357.14	19.99	13.33
24	338.15	352.67	14.52	24.79
27	343.55	393.30	49.75	21.83
30	348.65	369.54	20.89	13.17
33	351.65	391.13	39.48	20.83
36	353.15	420.11	66.96	29.74
39	358.65	381.40	22.75	36.69
42	364.15	399.97	35.82	35.03
45	368.15	395.21	27.06	19.43
48	369.15	371.09	1.94	12.96
51	370.15	389.19	19.04	12.92
54	371.15	400.34	29.19	19.26
57	373.15	404.25	31.10	20.17
60	379.15	413.15	34.00	14.38
63	383.15	397.72	14.57	18.48
66	387.15	400.82	13.67	25.96
69	392.15	399.95	7.80	18.09
72	394.15	438.05	43.90	15.16
75	395.65	416.78	21.13	17.70
78	406.15	430.32	24.17	22.49
81	412.65	390.31	-22.34	20.83
84	415.15	431.33	16.18	23.34
87	418.95	441.98	23.03	14.89
90	423.15	424.51	1.36	15.53
93	428.15	390.89	-37.26	21.07
96	432.65	352.07	-80.58	21.72
99	437.15	450.44	13.29	21.32
102	440.65	430.72	-9.93	15.96
105	446.15	440.16	-5.99	13.34
108	449.15	419.53	-29.62	22.75
111	453.15	393.92	-59.23	16.88
114	458.65	445.85	-12.80	13.82
117	461.65	452.29	-9.36	17.72
120	465.65	425.02	-40.63	17.80
123	472.15	439.80	-32.35	18.46
126	473.15	457.62	-15.53	13.50

Table SI5a. Single validation. Training set (100 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
1	303.15	305.94	2.79	7.68
3	308.15	308.23	0.08	11.57
4	310.15	307.14	-3.01	7.01
5	310.15	314.41	4.26	7.25
6	312.15	304.93	-7.22	5.97
7	313.65	318.18	4.53	6.77
8	314.15	308.35	-5.80	5.04
9	315.05	326.33	11.28	7.66
11	316.65	314.17	-2.48	9.20
12	317.65	327.25	9.60	10.37
14	320.15	323.16	3.01	12.66
15	324.15	316.34	-7.81	10.59
16	326.95	328.59	1.64	10.29
17	327.65	326.84	-0.81	8.14
18	330.65	347.31	16.66	16.19
19	332.15	327.70	-4.45	9.41
20	333.15	331.72	-1.43	10.19
21	337.15	348.64	11.49	15.50
24	338.15	338.21	0.06	7.25
25	342.15	355.11	12.96	16.74
27	343.55	366.84	23.29	15.47
28	344.15	353.63	9.48	11.09
30	348.65	364.45	15.80	13.00
31	350.15	352.86	2.71	13.10
32	351.15	347.61	-3.54	14.23
33	351.65	360.46	8.81	12.79
34	352.15	357.94	5.79	10.82
36	353.15	356.71	3.56	10.40
37	353.15	358.76	5.61	9.00
38	355.65	381.72	26.07	15.17
39	358.65	365.85	7.20	8.58
40	360.15	367.43	7.28	8.78
41	363.05	367.36	4.31	10.02
42	364.15	375.45	11.30	14.30
43	365.15	365.60	0.45	8.01
44	366.65	364.11	-2.54	11.29
45	368.15	366.78	-1.37	12.61
46	368.15	368.43	0.28	14.35
49	370.15	379.80	9.65	13.21
50	370.15	382.35	12.20	13.18
54	371.15	378.51	7.36	8.65
55	372.15	372.01	-0.14	13.19
56	372.65	368.75	-3.90	10.48

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
57	373.15	377.27	4.12	6.48
58	373.15	380.07	6.92	10.76
59	377.15	381.82	4.67	11.09
60	379.15	386.60	7.45	11.65
61	381.65	401.13	19.48	12.90
62	383.15	360.35	-22.80	12.00
65	384.15	392.47	8.31	9.47
66	387.15	383.95	-3.20	16.61
67	389.15	393.16	4.01	5.94
68	391.15	390.61	-0.54	10.99
69	392.15	387.30	-4.85	13.12
71	393.65	395.06	1.41	10.16
73	394.15	401.52	7.37	14.51
74	395.15	399.22	4.07	9.04
75	395.65	399.05	3.40	11.39
76	399.65	394.86	-4.79	9.36
78	406.15	413.91	7.76	9.19
79	406.15	407.38	1.23	10.17
81	412.65	407.94	-4.71	8.87
82	412.65	415.96	3.31	10.69
83	414.15	409.71	-4.44	14.43
84	415.15	418.83	3.68	14.67
85	417.15	421.20	4.05	11.85
86	417.15	427.34	10.19	11.48
87	418.95	421.41	2.46	12.11
88	420.15	422.25	2.10	8.49
89	422.15	423.32	1.17	12.01
90	423.15	426.12	2.97	12.32
93	428.15	399.47	-28.68	15.66
94	429.65	428.32	-1.33	10.01
95	429.65	437.04	7.39	14.05
96	432.65	413.56	-19.09	14.63
97	433.65	417.11	-16.54	9.29
98	436.15	428.63	-7.52	12.03
99	437.15	444.37	7.22	13.21
100	438.65	447.21	8.56	8.05
101	440.15	442.67	2.52	9.57
102	440.65	439.40	-1.25	9.61
103	442.15	437.85	-4.30	11.04
104	442.65	425.39	-17.26	10.81
105	446.15	441.27	-4.88	7.53
106	447.65	439.04	-8.61	10.76
107	448.15	416.95	-31.20	14.10
108	449.15	436.47	-12.68	9.38
109	451.15	438.88	-12.27	12.86
111	453.15	435.43	-17.72	13.44

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
112	456.65	441.27	-15.38	7.53
113	458.15	441.09	-17.05	16.02
114	458.65	459.06	0.41	9.09
116	461.15	445.14	-16.01	10.39
117	461.65	467.44	5.79	10.01
118	462.65	455.51	-7.14	9.53
119	463.65	452.77	-10.88	10.94
121	469.15	448.87	-20.28	16.36
122	471.65	464.04	-7.61	11.81
123	472.15	464.47	-7.68	10.69
126	473.15	466.92	-6.23	11.40

Table SI5b. Single validation. Test set (26 molecules). Results averaged over 16 trials (threshold: 50 K).

Name ID	experimental m.p. (K)	mean calc. m.p. (K)	mean error (K)	RMS (K)
2	308.15	328.47	20.32	9.77
10	315.65	315.38	-0.27	9.06
13	318.15	327.65	9.50	9.57
22	337.15	371.81	34.66	24.58
23	337.65	342.26	4.61	22.73
26	342.65	348.45	5.80	19.98
29	346.15	359.66	13.51	19.42
35	353.15	340.97	-12.18	17.18
47	368.65	398.09	29.44	15.94
48	369.15	373.86	4.71	23.10
51	370.15	381.99	11.84	18.52
52	370.65	352.44	-18.21	12.10
53	371.15	355.63	-15.52	25.96
63	383.15	414.52	31.37	20.59
64	383.15	422.66	39.51	16.31
70	393.15	409.83	16.68	29.55
72	394.15	445.27	51.12	18.78
77	400.65	382.34	-18.31	28.75
80	410.15	364.89	-45.26	16.44
91	426.65	417.64	-9.01	14.98
92	427.65	422.65	-5.00	11.01
110	452.15	446.17	-5.98	15.25
115	460.15	449.03	-11.12	15.05
120	465.65	428.39	-37.26	23.12
124	472.15	454.73	-17.42	13.09
125	472.15	437.07	-35.08	24.79