Supplementary material

Fusion property dataset of compounds with one acid and one or more other (carbonyl, hydroxyl, acid) functionalities

If in the original reference multiple transition points were given, always the sum over all transition points is taken. If in the original reference a range for T_{fus} was given, the middle point is taken.

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
hydroxy mono-acids							
2-hydroxy acetic		OC(=O)CO	351.3	19.3	[1]	338	14.9
(glycolic)			352.65		Lide†		
2-hydroxy propanoic	*dl*	OC(=O)C(O)C	289.9	11.34	AC (Domalski)	338	14.9
(lactic)	S		330.4	16.05	[2]		
			290		NIST (Wilhoit)†		
	d		326.15		Lide†		
	l		298.65		Lide†		
2-hydroxy butanoic		OC(=O)C(O)CC	317.35		Lide	330	16.7
3-hydroxy butanoic		OC(=O)CC(O)C	322.15		Lide	330	16.7
2-hydroxy-2-methyl-		OC(=O)C(C)(O)C	354		NIST (Emmons)	338	14.9
propanoic (acetonic)							
1-hydroxy-1-cyclo-		OC(=O)C1(O)CC1	382.15		Aldrich	343	14.0
propanecarboxylic							
2-hydroxy pentanoic		OC(=O)C(O)CCC	307.15		Lide	324	18.5
2-hydroxy-2-methyl butanoic		OC(=O)C(O)(C)CC	347.15		Aldrich	330	16.7
2-hydroxy-3-methyl butanoic	(*S*)-(+)	OC(=O)C(O)C(C)C	342.15		Aldrich	330	16.7
			359.6		Aldrich		
2-hydroxy hexanoic		OC(=O)C(O)CCCC	333.15		Lide	319	20.3
2-hydroxy-4-methyl-		OC(=O)C(O)CC(C)C	354.65		Lide	324	18.5
pentanoic (leucic)							
2-hydroxy-3,3-dimethyl-		OC(=O)C(O)C(C)(C)C	322.15		Aldrich	330	16.7
butanoic							
2-hydroxy octanoic		OC(=O)C(O)CCCCCC	343.15		Lide	312	23.9
2-(1-hydroxycyclohexyl)-		OC1(C(C(=O)O)CC)CCCCC1	354.65		Lide	327	17.6

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
butanoic (cyclobutyrol)							
3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic		OC(=O)C(CO)(C)CO	463.15		Lide	371	30.0
2,3,4,5,6-pentahydroxy-hexanoic (gluconic)		OC(=O)C(O)C(O)C(O)C(O)C(O)CO	404.15		Lide	412	68.3
oxo mono-acids							
oxo acetic (glyoxilic)		OC(=O)C=O	371.15		Lide	343	14.0
2-oxo propanoic (pyruvic)		OC(=O)C(=O)C	286.95		Lide	343	14.0
2-oxo butanoic		OC(=O)C(=O)CC	306.15		Lide	334	15.8
2-oxo pentanoic		OC(=O)C(=O)CCC	279.65		Lide	327	17.6
4-oxo pentanoic (levulinic)		OC(=O)CCC(=O)C	306.2	9.22	NIST (Acree)	327	17.6
3-methyl-2-oxo butanoic		OC(=O)C(=O)C(C)C	304.65		Lide	334	15.8
5-oxo hexanoic		OC(=O)CCCC(=O)C	286.65		Lide	322	19.4
4-methyl-2-oxo pentanoic		OC(=O)C(=O)CC(C)C	283.15		Lide	327	17.6
3,3-dimethyl-2-oxo butanoic		OC(=O)C(=O)C(C)(C)C	363.65		Lide	334	15.8
3-oxo-1-cyclo-pentanecarboxylic		OC(=O)C1CC(=O)CC1	333.65		Aldrich	343	14.0
6-oxo heptanoic		OC(=O)CCCCC(=O)C	313.15		Lide	317	21.2
2-oxo cyclopentane acetic		OC(=O)CC1C(=O)CCC1	321.65		Aldrich	334	15.8
camphocarboxylic		CC1(C2CCC1(C(=O)C2C(=O)O)C)C	400.65		Lide	338	14.9
2-oxo octanoic		OC(=O)C(=O)CCCCCC	307.65		Aldrich	314	23.0
7-oxo octanoic		OC(=O)CCCCCC(=O)C	301.15		Aldrich	314	23.0
pinonic		CC1(C(CC1C(=O)C)CC(=O)O)C	377.8	23.8	[3]	330	16.7
odd linear diacids							
malonic		OC(=O)CC(=O)O	406	18.739	[4]	401	19.6

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{\mathrm{fus}}}{\mathrm{K}}$ (exp.)	$\frac{\Delta H_{\mathrm{fus}}}{\mathrm{kJmol^{-1}}}$ (exp.)	Ref.	$\frac{T_{\mathrm{fus}}}{\mathrm{K}}$ (est.)	$\frac{\Delta H_{\mathrm{fus}}}{\mathrm{kJmol^{-}}}$ (est.)
			407.46	23.1	[5]†		
			408.6		[6]†		
			408		NIST (Wilhoit)†		
glutaric		OC(=O)CCCC(=O)O	369	22.043	[4]	375	23.2
			368.48	23.36	[7]†		
			361.2	21.1	[8]†		
			370.2		[6]†		
pimelic		OC(=O)CCCCCC(=O)O	366.23	25.2	[8]	358	26.8
			377.1	28.95	[7]†		
			378.4		[6]†		
azelaic		OC(=O)CCCCCCCC(=O)O	371.56	30.410	[8]	346	30.4
			380.0	32.68	[7]†		
			375.6	35.3	AC (Chen)†		
			381.2		[6]†		
even linear diacids							
oxalic		OC(=O)C(=O)O	370	3.424	[4]‡	499	30.1
			462.65		[9]‡		
			464.45		NIST (Wilhoit)‡		
succinic		OC(=O)CCC(=O)O	458	31.259	[4]	459	33.7
			457	32.95	[7]†		
			455.2	34.03	[8]†		
			457.2		[10]†		
adipic		OC(=O)CCCCC(=O)O	423	35.891	[4]	432	37.3
			425.5	34.85	[7]†		
			419.0†	33.7	[8]†		

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
suberic		OC(=O)CCCCCCC(=O)O	407.94	41.8	[8]	412	41.0
			413.5†	38.20	[7]†		
			415.3	28.82	NIST (Acree)&		
sebacic		OC(=O)CCCCCCCCC(=O)O	403.59	47.0	[8]	396	44.6
			404.0	40.81	[7]†		
			405.7	46.9	AC (Ventola)†		
			405.6	45.3	AC (Xia)†		
branched noncyclic diacids							
methyl malonic		OC(=O)C(C)C(=O)O	403	30.746	[4]	401	19.6
			408		[11]†		
			407.5		[12]†		
methyl succinic		OC(=O)C(C)CC(=O)O	383	9.980	[4]	387	21.4
			388.4		[10]†		
			383		[11]†		
			388.15		Lide†		
ethyl malonic		OC(=O)C(CC)C(=O)O	385.8		[12]	387	21.4
			384		NIST (Vogel)†		
			387.15		Lide†		
dimethyl malonic		OC(=O)C(C)(C)C(=O)O	464.6 (dec)		[12]	401	19.6
			465.65		Lide†		
2-methyl glutaric		OC(=O)C(C)CCC(=O)O	349	30.259	[4]	375	23.2
			352.6		[10]†		
3-methyl glutaric		OC(=O)CC(C)CC(=O)O	356	27.351	[4]	375	23.2
			356		[11]†		
			360.15		Lide†		

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
2,2-dimethyl succinic		OC(=O)C(C)(C)CC(=O)O	414.2		[10]	387	21.4
			372		[11]*		
			408-414		NIST (several ref)†		
3-methyl adipic		OC(=O)CC(C)CCC(=O)O	367		[11]	366	25.0
butyl malonic		OC(=O)C(CCCC)C(=O)O	377.2		[12]	366	25.0
			377.65		Lide†		
2,2-dimethyl glutaric		OC(=O)C(C)(C)CCC(=O)O	356.6		[10]	375	23.2
			413		NIST (Allinger)		
3,3-dimethyl glutaric		OC(=O)CC(C)(C)CC(=O)O	377		[11]	375	23.2
			376.65		Lide†		
diethyl malonic		OC(=O)C(CC)(CC)C(=O)O	400.15		Lide	375	23.2
tetramethyl succinic		OC(=O)C(C)(C)C(C)(C)C(=O)O	406	19.9	AC (Domalski)	387	21.4
cyclic diacids							
1,1-cyclopropane dicarboxylic		O=C(O)C1(C(=O)O)CC1	413	17.4	[3]	410	18.7
			413.65		Lide†		
1,1-cyclobutane dicarboxylic		O=C(O)C1(C(=O)O)CCC1	433.2	16.9	[3]	410	18.7
			431.15		Lide†		
1,2-cyclopentane dicarboxylic		O=C(O)C1C(C(=O)O)CCC1	428.6	19.1	[3]	410	18.7
1,3-cyclohexane dicarboxylic		O=C(O)C1CC(C(=O)O)CCC1	439.0	12.9	[3]	410	18.7
1,4-cyclohexane dicarboxylic	*trans*	O=C(O)C1CCC(C(=O)O)CC1	585.65		Lide	410	18.7
norpinic	*trans*	O=C(O)C1CC(C(=O)O)C1(C)C	410		[13]	410	18.7
pinic		CC1(C(CC1C(=O)O)CC(=O)O)C	343		[13]	393	20.5
1,2,2-trimethyl-1,3-cyclopentanedicarboxylic (camphoric)	(±)	O=C(O)C1CCC(C(=O)O)(C)C1(C)C	475.15		Lide	410	18.7

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
keto diacids							
oxo succinic		OC(=O)C(=O)CC(=O)O	437	50.382	[4]	422	32.0
			434		[14]†		
2-oxo glutaric		OC(=O)C(=O)CCC(=O)O	386	34.693	[4]	410	33.8
			388.7	28.59	AC (Contineanu)		
			388		[14]†		
			389.65		NIST (Wilhoit)†		
3-oxo glutaric		OC(=O)CC(=O)CC(=O)O	397	45.895	[4]	410	33.8
			405		[14]†		
2-oxo adipic		OC(=O)C(=O)CCCC(=O)O	397.15		LookChem	401	35.6
3-oxo adipic		OC(=O)CC(=O)CCC(=O)O	398.15		Aldrich	401	35.6
4-oxo pimelic		OC(=O)CCC(=O)CCC(=O)O	416		[14]	392	37.4
5-oxo azelaic		OC(=O)CCCC(=O)CCCC(=O)O	381		Aldrich	378	41.0
hydroxy di- and triacids							
2-hydroxy malonic (tartronic)		OC(=O)C(O)C(=O)O	428	30.619	[4]	428	31.1
hydroxy succinic (malic)		OC(=O)C(O)CC(=O)O	403	29.031	[4]	416	32.9
	dl		402	33.522	NIST (Ceolin)† , AC (Domalski)†		
	dl		396	30.17	NIST (Ceolin)† , AC (Domalski) †		
	d		376	23.01	AC (Leclercq)		
	l		372.7		NIST (Wilhoit) †		
2-methyl-2-hydroxy succinic		OC(=O)C(O)(C)CC(=O)O	379	35.697	[4]	416	32.9
3-hydroxy-3-methylglutaric		OC(=O)CC(O)(C)CC(=O)O	379.7		Aldrich	405	34.7
tartaric		OC(=O)C(O)C(O)C(=O)O	480	62.723	[4]	432	44.5

Table S1: experimental and estimated fusion data of functionalized acids.

name	stereo-info	SMILES	$\frac{T_{fus}}{K}$ (exp.)	$\frac{\Delta H_{fus}}{kJmol^{-1}}$ (exp.)	Ref.	$\frac{T_{fus}}{K}$ (est.)	$\frac{\Delta H_{fus}}{kJmol^{-}}$ (est.)
	d		445.1	32.2	NIST, AC (Mura)		
citric		OC(=O)CC(O)(C(=O)O)CC(=O)O	427	43.455	[4]	446	51.0
			427.15		NIST (Wilhoit)†		
isocitric		OC(=O)C(O)C(C(=O)O)CC(=O)O	378.15		Lide	446	51.0
tetrahydroxy adipic	glucaric	OC(=O)C(O)C(O)C(O)C(O)C(=O)O	398.65		Lide	434	71.2
	galactaric		528.15 (dec)		Lide		
tri- and tetra-acids							
1,2,3-propane tricarboxylic		OC(=O)CC(C(=O)O)CC(=O)O	439.15		Lide	436	39.4
butane tetracarboxylic		OC(=O)CC((=O)O)C((=O)O)CC(=O)O	509.65		Lide	478	53.8
			469 (dec)		Aldrich		

†. Not taken into account because it is quite close to other data points of the molecule already taken into account. $T_{\text{fus}}, \Delta H_{\text{fus}}$ couples have prevalence over single T_{fus} points.

&. Not taken into account, because by comparison with other data, it seems that lower transition points were overlooked.

$*$. Not taken into account because it contradicts with several other T_{fus} of the same molecule.

‡. Not taken into account because it is unclear if the low T_{fus} of Booth (2010) is due to a solid-solid transition, or if the widely different T_{fus} are due to dimorphism.

(dec). The molecule undergoes decomposition at this temperature, hence the true melting point will probably be higher.

Notations for secondary data sources: Aldrich [15], Lide [16], LookChem [17], AC (=Acree-Chickos (2010)) [18], NIST [19]. For the last two, the first author of the original data source is given in brackets.

Table S2. Experimental $\omega_{ls}(298\,\text{K}, \Delta C_{p,ls} = 0)$ and estimated (with experimental T_{fus} and the ΔH_{fus} estimation method developed in this work).

name	exp. ω_{ls}	est. ω_{ls}
glycolic	0.51	0.40
lactic (S)	0.28	0.26
lactic (*dl*)	-0.06	-0.07
2-hydroxybutanoic	n/a	0.18
3-hydroxybutanoic	n/a	0.22
acetonic	n/a	0.41
1-hydroxy-1-cyclopropane carboxylic	n/a	0.54
2-hydroxypentanoic	n/a	0.1
2-hydroxy-2-methyl butanoic	n/a	0.41
2-hydroxy-3-methyl butanoic (*S*)	n/a	0.38
2-hydroxy-3-methyl butanoic	n/a	0.50
2-hydroxy hexanoic	n/a	0.38
leucic	n/a	0.52
2-hydroxy-3,3-dimethyl butanoic	n/a	0.22
2-hydroxy octanoic	n/a	0.55
cyclobutyrol	n/a	0.49
3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic	n/a	1.88
gluconic	n/a	3.15
glyoxilic	n/a	0.48
pyruvic	n/a	-0.09
2-oxobutanoic	n/a	0.074
2-oxopentanoic	n/a	-0.20
levulinic	0.04	0.083
3-methyl-2-oxobutanoic	n/a	0.06
5-oxohexanoic	n/a	-0.13
4-methyl-2-oxopentanoic	n/a	-0.16

name	exp. ω_{ls}	est. ω_{ls}
3,3-dimethyl-2-oxobutanoic	n/a	0.50
3-oxo-1-cyclopentanecarboxylic	n/a	0.26
6-oxoheptanoic	n/a	0.18
2-oxocyclopentane acetic	n/a	0.20
camphocarboxylic	n/a	0.67
2-oxooctanoic	n/a	0.13
7-oxooctanoic	n/a	0.04
pinonic	0.88	0.62
malonic	0.87	0.91
glutaric	0.74	0.78
pimelic	0.82	0.88
azelaic	1.06	1.06
succinic	1.91	2.07
adipic	1.86	1.93
suberic	1.97	1.93
sebacic	2.16	2.04
methylmalonic	1.40	0.89
methylsuccinic	0.39	0.83
ethylmalonic	n/a	0.
dimethylmalonic	n/a	1.23
2-methylglutaric	0.78	0.59
3-methylglutaric	0.78	0.66
2,2-dimethylsuccinic	n/a	1.05
3-methyladipic	n/a	0.82
butylmalonic	n/a	0.92
2,2-dimethylglutaric	n/a	0.67
2,2-dimethylglutaric	n/a	1.13
3,3-dimethylglutaric	n/a	0.85
diethylmalonic	n/a	1.04
tetramethylsuccinic	0.93	1.00
1,1-cyclopropane dicarboxylic	0.85	0.91
1,1-cyclobutane dicarboxylic	0.92	1.02
1,2-cyclopentane dicarboxylic	1.02	1.00
1,3-cyclohexane dicarboxylic	0.73	1.05
1,4-cyclohexane dicarboxylic	n/a	1.61
norpinic	n/a	0.89
pinic	n/a	0.47
camphoric	n/a	1.22
oxosuccinic	2.81	1.79
2-oxoglutaric	1.39	1.35
2-oxoglutaric	1.17	1.39
3-oxoglutaric	2.01	1.48
2-oxoadipic	n/a	1.56
3-oxoadipic	n/a	1.57
4-oxopimelic	n/a	1.86

name	exp. ω_{ls}	est. ω_{ls}
5-oxoazelaic	n/a	1.57
tartronic	1.63	1.66
malic	1.33	1.50
malic (d)	0.84	1.20
2-methyl-2-hydroxysuccinic	1.34	1.23
3-hydroxy-3-methylglutaric	n/a	1.31
tartaric	4.17	2.96
tartaric (d)	1.87	2.58
citric	2.30	2.70
isocitric	n/a	1.89
glucaric	n/a	3.15
galactaric	n/a	5.44
1,2,3-propanetricarboxylic	n/a	2.22
butane tetracarboxylic (Lide)	n/a	3.92
butane tetracarboxylic (Aldrich)	n/a	3.44

n/a: No experimental value available.

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