Table I. Observed and predicted melting point values of the dataset studied.

Substances	Set	Mp _{obs}		Mp _{pred II}		
Substances	361	(°C)	Mp _{pred I} (°C)	(°C)	Mp _{pred III} (°C)	Mp _{pred IV} (°C)
buramate	tr	40				111.7
fenpiprane		41	87.5			
trimipramine	tr	45				
•	te	48				
phencarbamide	tr	48 51	132.9			
banactyzine	tr	53				
ethopropazine	te					
xibenolol	tr	57				
prometazine	tr	60				
gemfibrozil	tr	61	76.2			
isosorbide	te	61	213.6			
fluanisone	tr	67.5				
penbutolol	te	68				
ranitidine	tr	69				
propoxyphene	tr	75				
novonal	tr	75				
phenadoxone	te	75				
ibuprofen	tr	75				
mebutamate	te	77				
moxaverine	tr	78				
etisazol	tr	78				
nabumetone	te	80				118.0
cloranolol	tr	82				
pentifylline	tr	82				
fentanyl	te	83				
zipeprol	tr	83				
anileridine	tr	83				
amphetaminil	te	85				
piprozolin	tr	86				
econazole	tr	86.8				
chloroquine	tr	87				
methdilazine	te	87				
noxythiolin	tr	. 88				130.2
tulobuterol	te	89				
acetorphan	tr	89				
zotepine	te	90				
vinylbital	tr	90				
phenindamine	tr	91				
carisoprodol	tr	92				
alclofenac	tr	92				124.4
maprotiline	te	92				
tolindate	te	94				
perphenazine	tr	94				
ketoprofen	tr	94				
thenaldine	te	95				
alibendol	tr	95			148.9	
tamoxifen	tr	96				
tropicamide	tr	96	110.6	141.8	121.2	124.5

limaprost	te	97	125.4	102.2	105.1	110.9
metaproterenol	tr	100	93.1	113.0	126.4	110.8
medmain	tr	100	123.6	117.7	131.0	124.1
plafibride	te	100	149.1	135.7	136.9	140.6
acetylpheneturide	tr	100	127.1	123.6	150.0	133.6
phenocoll	tr	100.5	143.1	114.6	140.0	132.6
hycanthone	te	100.6	145.7	171.9	162.6	160.1
piperidione	tr	102	120.8	151.6	120.7	131.0
isoxsuprine	tr	102.5	94.6	93.0	94.6	94.1
meprobamate	te	104	109.9	164.1	126.5	133.5
diphemethoxidine	tr	106	113.8	132.1	106.5	117.5
pipobroman	tr	106	114.5	163.6	109.2	129.1
mepiprazole	tr	106	127.1	119.1	138.1	128.1
zidovudine	te	106	143.5	115.9	238.8	166.1
bupivacaine	tr	107	84.0	104.6	83.5	90.7
cetoxime	te	107	125.9	154.2	125.9	135.3
toremifene	tr	108	93.0	158.1	93.8	115.0
acecarbromal	tr	109	145.2	125.3	133.1	134.5
celiprolol	tr	110	85.3	163.6	99.2	116.0
flurbiprofen	te	110	132.8	106.0	132.4	123.7
amphotalide	tr	113	143.3	130.3	146.0	139.9
valnoctamide	te	113.5	71.6	97.4	67.9	79.0
isbogrel	te	114	104.1	148.4	110.8	121.1
ifenprodil	tr	114	131.2	101.5	112.7	115.1
atropin	tr	114	117.9	180.0	121.5	139.8
detomidine	tr	114	133.7	153.0	138.5	141.7
bamipine	· tr	115	88.3	159.0	86.1	111.1
flupirtine	tr	115	141.3	121.1	152.6	138.3
ipriflavone	te	115	176.4	143.1	177.5	165.7
flumetramide	tr	115.5	103.8	155.4	151.4	136.9
dibenzepin	tr	116	132.5	124.7	153.5	136.9
valsartan	tr	116	159.5	135.5	159.8	151.6
pericyazine	te	116	152.2	140.5	160.8	151.2
fadrozole	te	117	173.7	145.4	177.3	165.5
moperone	tr	118	151.4	133.8	104.1	129.8
flutoprazepam	tr	118	166.2	167.1	159.9	164.4
morphazinamide	te	118.5	175.4	152.6	166.0	164.7
acebutolol	tr	119	108.3	105.1	101.5	105.0
terbutaline	te	119	120.4	152.2	120.2	131.0
pirozadil	tr	119	152.0	120.2	174.3	148.8
chlophedianol	tr	120	95.7	115.3	84.1	98.4
pridinol	tr	120	91.9	143.8	86.5	107.4
antazoline	tr	120	102.5	126.9	103.7	111.0
vinconate	te	120	243.1	148.1	197.1	196.1
capobenic acid	tr	121	111.9	148.4	116.8	125.7
difenpiramide	tr	122	119.4	157.1	140.1	138.9
propizepine	te	122	111.7	121.4	170.7	134.6
benzoic acid	tr	122.4	135.7	179.3	167.2	160.7
bamethan	te	123.5	70.9	96.3	88.4	85.2
nadolol	tr	124	159.7	136.7	123.4	139.9

benzarone	tr	. 124.3	185.5	186.0	184.4	185.3
lofexidine	tr	126	132.4	158.9	106.0	132.5
mecloqualone	te	126	187.1	144.3	182.4	171.3
seratrodast	tr	128	168.5	134.4	108.0	137.0
simetride	te	128	103.5	138.7	133.9	125.4
febantel	tr	129	121.3	132.0	175.6	143.0
clonidine	tr	130	112.8	152.4	130.0	131.7
xylometazoline	te	131	93.5	148.7	86.5	109.5
thozalinone	tr	133	145.5	142.1	145.8	144.5
erytromycin	tr	135	159.3	129.0	152.6	147.0
mephenytoin	te	136	128.0	132.9	135.7	132.2
aminorex	tr	136	155.3	110.0	157.0	140.8
praziquantel	tr	136	179.7	165.0	170.9	171.8
ipsapirone	te	137	169.7	151.0	170.4	163.7
butalbital	tr	138	142.8	157.8	140.3	146.9
zafirlukast	tr	138	177.1	165.4	193.5	178.7
alizapride	tr	139	192.9	182.0	189.3	188.1
phenazopyridine	te	139	183.5	145.7	193.4	174.2
alpidem	tr	140	115.6	155.4	132.3	134.4
erythrocentaurin	te	140	185.6	149.6	184.1	173.1
cimetidine	tr	141	147.7	125.2	137.3	136.8
ethinylestradiol	tr	141	102.6	124.0	179.2	135.2
letosteine	tr	142	163.5	153.5	106.0	141.0
proglumide	te	142	103.9	127.1	118.7	116.6
fexofenadine	te	142	115.0	144.2	120.4	126.5
carbaryl	tr	142	174.6	137.5	162.2	158.1
acetylsalicylic acid	tr	142.4	144.6	156.6	176.4	159.2
ahistan	tr	144	171.4	127.8	156.1	151.8
carbutamide	tr	144	137.3	178.2	158.4	158.0
doxofylline	te	144	181.2	158.4	220.0	186.5
felodipin	tr	145	100.5	143.2	138.8	127.5
atenolol	tr	146	132.0	142.2	113.2	129.1
sertaconazole	tr	146	148.8	155.3	138.5	147.5
ketoconazol	te	146	191.3	152.3	184.4	176.0
metoclopramide	tr	146.5	109.7	138.2	109.8	119.2
pyrinoline	te	146.5	174.5	155.9	178.5	169.6
clotrimazole	tr	147	143.2	138.3	153.6	145.0
haloperidol	tr	148	152.1	132.3	105.4	130.0
thialbarbital	tr	148	152.2	146.9	134.1	144.4
salacetamide	te	148	166.8	165.5	172.6	168.3
dimecrotic acid	te	149	176.3	133.8	147.4	152.5
morazone	tr	149	141.1	121.0	149.6	137.2
aceclofenac	tr	149	158.4	177.6	154.3	163.4
astemizole	te	149.1	148.6	143.4	167.5	153.2
abecarnil	tr	150	222.2	181.4	198.0	200.5
acemetacin	tr	150	184.9	201.8	203.5	196.7
felbamate	tr	151	166.9	154.0	165.3	162.1
mafenide	te	151	234.3	130.6	195.4	186.8
ujothion	te	152	140.2	152.3	134.2	142.2
naproxen	tr	152	161.8	153.6	155.3	156.9

glymidine	tr	152	105.8	174.4	160.5	146.9
bufexamac .	tr	153	152.3	147.5	116.0	138.6
florfenicol	tr	153	158.1	168.5	147.9	158.2
testosterone	te	153	180.2	203.4	181.9	188.5
taurolidine	tr	154	185.1	189.7	189.0	187.9
vamicamide	te	156	146.4	143.3	105.2	131.6
ketobemidone	tr	156	160.5	169.3	106.5	145.4
amobarbital	te	156	116.7	168.1	131.8	138.8
erdosteine	tr	156	161.1	116.7	135.9	137.9
benzetimide	te	156	122.1	151.9	146.3	140.1
urapidil	tr	156	171.7	127.9	147.3	149.0
metizoline	tr	156	163.3	130.5	148.6	147.4
omeprazole	tr	156	148.5	144.0	162.8	151.8
phenallymal	tr	156	151.6	160.3	176.1	162.7
moricizine	te	156	201.5	204.9	187.5	198.0
zileuton	te	157	186.1	182.1	186.9	185.0
succisulfone	tr	157	188.7	201.3	191.4	193.8
salicylic acid	tr	157	181.5	210.8	191.4	195.6
dapiprazole		158				
lidoflazine	tr	158	121.6 140.8	107.7	155.0	128.1
amidephrine	te	159		126.4	100.3	122.5
adrafinil	tr		122.2	163.6	146.0	143.9
	tr	159	130.0	173.8	153.4	152.4
azacyclonol bucetin	tr	160	111.4	118.9	115.5	115.3
methallatal	te	160	168.1	146.0	124.5	146.2
	tr	160	125.2	124.4	127.1	125.5
benzydamine	tr	160	135.7	146.8	127.3	136.6
oxaprozin	te	160.5	110.9	132.5	175.0	139.5
warfarin	tr	161	186.9	221.6	191.7	200.0
propranolol	tr	162	155.2	162.1	108.5	141.9
torsemide	te	163	179.1	135.4	163.9	159.5
famotidine	tr	163	150.3	127.3	176.7	151.4
tyramine	tr	164	163.4	154.1	132.1	149.8
tolrestat	tr	164	138.5	158.6	143.2	146.8
modafinil	tr	164	151.9	168.0	144.2	154.7
halazepam	te	164	174.1	146.2	162.6	161.0
guanoxan	tr	164	195.1	181.6	186.6	187.8
Metralindole	te	164	210.7	204.0	196.0	203.6
lorazepam	tr	166	186.2	183.5	199.1	189.6
fosfosal	te	168	230.5	230.6	247.4	236.2
sumatriptan	te	169	164.1	148.6	142.9	151.9
acetaminophen	tr	169	174.3	164.2	152.7	163.7
glyburide	tr	169	177.9	171.0	156.7	168.5
pindolol	tr	170	156.0	138.6	139.2	144.6
tolazamide	te	170	151.7	175.8	157.2	161.6
benperidol	tr	170	151.1	141.8	161.7	151.6
metopimazine	tr	170	173.8	153.7	178.9	168.8
isoniazid	tr	171.4	195.6	210.3	197.0	201.0
heptabarbital	te	174	177.0	117.9	155.8	150.2
piposulfan	tr	175	182.2	156.4	171.9	170.1
amisometradine	tr	175	184.8	169.3	174.4	176.2

mephobarbital	te	176	149.6	138.6	156.9	148.4
acifran	tr	176	183.4	180.7	187.0	183.7
propallylonal	tr	177	200.7	167.7	146.9	171.7
ximoprofen	te	178	153.3	169.1	144.3	155.6
sulpiride	tr	178	180.6	158.7	158.0	165.7
zomepirac	tr	178	189.0	160.2	166.4	171.9
nomifensine	te	179	147.3	173.0	139.2	153.2
dextromoramide	tr	180	114.8	105.0	109.6	109.8
molindone	tr	180	149.6	107.0	162.1	139.6
sulthiame	te	180	182.4	130.1	187.3	166.6
irbesartan	tr	180	175.9	114.7	192.2	160.9
letrozole	tr	181	229.2	131.2	198.4	186.3
amphenidone	te	182.5	183.8	166.2	183.9	177.9
zoxazolamine	tr	184	191.3	162.9	224.4	192.8
haloxazolam	tr	185	187.6	173.9	187.6	183.0
bezafibrate	tr	186	157.1	149.8	133.5	146.8
oxazolam	te	186	218.7	128.1	183.0	176.6
acetoaminosalol	tr	187	178.4	148.9	173.0	166.8
acetohexamide	te	188	176.9	176.8	166.4	
verazide	te	189	170.5	140.5	165.3	173.4 158.8
glisoxepid	tr	189	133.8	153.6	178.5	155.3
pyrazinamide	tr	189	191.7	161.3	211.5	
spiperone	tr	190	169.7	178.2		188.2
carbamazepine	tr	190	209.3	170.2	146.7	164.9
glibornuride	te	190	119.0	170.8	212.4	197.5
clebopride		194	132.9		168.4	148.9
acediasulfone	tr tr	194	183.9	139.1	151.4	141.1
hymecromone		194	185.1	152.8	192.9	176.5
aceglutamide	te	194	154.5	164.8	222.0	190.6
zopolrestat	tr tr	197		169.6	154.5	159.5
probenecid	tr te	197	160.5 177.3	163.9	223.8	182.8
piroxicam		198	214.2	169.1	127.6	158.0
furonazide	tr •-	198	214.2	160.8	221.4	198.8
ursodiol	tr te	203	121.6	156.3	185.2	188.1
caroxazone		203		149.0	167.0	145.9
	tr +-	205	197.8	178.8	194.0	190.2
oxazepam lonidamine	tr		185.3	125.7	202.3	171.1
indoramin	te	207	193.3	111.0	189.4	164.6
albendazole	tr •-	208	145.0	159.0	163.8	155.9
vigabatrin	tr	208	156.3	176.5	165.6	166.1
buprenorphine	te	209	128.6	179.4	118.6	142.2
• •	tr	209	193.6	168.9	201.2	187.9
albutoin methetion	tr	210	114.0	136.5	100.1	116.9
	te	210	92.7	148.6	140.4	127.2
griseofulvin	tr	219	200.9	195.7	206.5	201.1
tirofiban	te	223	179.0	117.9	115.9	137.6
hydrocortisone	tr	223	207.8	197.5	209.9	205.0
Melengestroleacetate	tr	224	224.5	182.1	183.9	196.8
delavirdine	tr	226	200.9	215.8	187.1	201.3
acitretin	tr	228	117.8	155.8	119.7	131.1
apazone	te	228	135.3	178.1	173.9	162.4

oxibendazole	tr	230	190.1	211.6	184.9	195.5
ondansetron	te	231	246.8	154.7	190.6	197.4
ubenimex	te	233	134.4	165.4	138.4	146.1
phenopyrazone	tr	233	169.0	102.3	167.7	146.4
diaveridine	tr	233	165.4	117.2	168.9	150.5
chlorazanil	tr	233	166.5	152.1	175.3	164.6
sulfamerazine	tr	234	196.8	188.6	191.7	192.4
yohimbine	te	234	186.2	180.6	239.8	202.2
lotrifen	tr	238	199.7	194.4	199.2	197.8
zolimidine	te	242	166.1	149.4	179.1	164.9
clometacin	tr	242	187.8	196.0	190.9	191.5
velnacrine	tr	245	197.4	186.0	195.0	192.8
arprinocid	tr	245	198.5	182.8	210.7	197.3
metolazone	te	252	201.5	183.2	200.7	195.1
flumequine	tr	253	225.6	216.1	219.1	220.3
aciclovir	tr	255	237.1	182.1	242.0	220.4
skf105657	te	257	197.7	180.7	184.1	187.5
ciprofloxacin	tr	266	213.9	202.5	219.9	212.1
hydrochlorothiazide	tr	267	258.5	196.4	253.5	236.1
ibafloxacin	tr	269	222.8	189.5	212.3	208.2
pazufloxacin	te	269	243.0	190.2	249.0	227.4
theophylline	tr	270	253.5	210.9	242.9	235.8
acefylline	te	271	254.8	182.9	241.7	226.5
hydroflumethiazide	tr	272	257.4	234.2	252.3	248.0
moxesterol	tr	280	193.5	228.2	184.5	202.1
primidone	te	281	200.3	146.3	149.1	165.3
prazosin	tr	285	227.4	184.1	226.9	212.8
acedapsone	tr	289	175.3	136.6	171.5	161.1
phenytoin	te	295	189.2	133.9	173.0	165.3
orotic acid	tr	345	275.9	263.2	298.4	279.2

The dataset is presented as training (tr) and test (te) sets. Mp_{obs} and Mp_{pred} denotes observed

and predicted mp, respectively. Model I is based on 2D descriptors, model II on 3D descriptors, model III on both 2D and 3D descriptors and model IV is the averaged consensus of

the three developed models.