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Table SM1. High-temperature hydrocarbon compounds with their experimental and calculated AIT values.

Compound Name	Exp. AIT (°C)	Calc. AIT (°C) Type 1	Calc. AIT (°C) Type 2	Calc. AIT (°C) Type 3
2,2-Dimethylbutane	435	435	413	423
2-Methylbutane	420	410	392	399
Butylbenzene[b]	410	408	405	393
1-Butene	440	402	407	393
Propane	470	438	455	448
Ethenylbenzene	490	475	468	465
Benzene[a]	555	550	558	553
Bicyclo(2.2.1)hepta-2,5-diene	350	386	381	361
3,3-Dimethyl-1-butyne[a]	390	379	383	391
2,3-Dimethyl-2-butene	400	429	434	411
2,4,4-Trimethyl-1-pentene	415	409	388	413
1,2-Dimethylbenzene	465	498	469	482
Ethane[b]	515	475	503	505
1-Ethyl-2-Methylbenzene	440	451	433	433
1,4-Dimethylbenzene	525	513	519	521
1-Methylnaphthalene[a]	485	511	523	486
1,3-Diethyl-5-methylbenzene	455	408	444	446
1,2,4-Trimethylbenzene	485	483	482	495
2,2,4,6,6-Pentamethylheptane	430	423	442	434
Naphthalene	540	552	556	540
Ethene	425	439	442	442
2,2,3,3-Tetramethylpentane	430	430	430	430
1,3-Butadiene[b]	415	402	408	404
2,3-Dimethyl-1-butene	360	385	378	373
1,3,5-Trimethylbenzene	550	514	526	524
Cyclopropane	495	438	479	498
1-Ethyl-3-methylbenzene	480	469	469	471
2-Ethyl-1,1'-biphenyl	440	427	452	455
Ethylbenzene	430	484	481	468
1,3-Diethylbenzene	450	419	416	419
2,3,3,4-Tetramethylpentane	430	432	437	431
1,1'-Biphenyl	540	518	534	531
(1-Methylpropyl)benzene	415	425	401	412
Butane	365	401	414	404
3-Ethyl-2,4-dimethylpentane	390	382	383	367
1,2,3,4-Tetrahydronaphthalene[a]	390	393	385	424
1,2,3-Trimethylbenzene	470	472	468	461
(2-Methylpropyl)benzene	425	455	447	461
2,3,3-Trimethyl-1-butene	375	373	401	395
3-Methyl-1-butene	365	398	380	377
1,4-Diethylbenzene	430	417	414	419
2,2,3-Trimethylbutane	450	437	450	428
2,3,3-Trimethylpentane	425	422	412	419
2,2,3-Trimethylpentane	430	420	411	424
2,2,4-Trimethylpentane	410	452	424	439
1-Ethylnaphthalene[b]	480	460	487	453
2,3-Dimethylbutane	415	415	416	415
1-Ethyl-4-methylbenzene	475	465	463	472
Methylbenzene[b]	535	532	543	532
1,2-Diethylbenzene	380	400	400	399
1,3-Dimethylbenzene	525	520	530	522

[a]Cross-validation set compound [b]Prediction set compound

Table SM2. Nitrogen compounds with their experimental and calculated AIT values.

Compound Name	Exp. AIT (°C)	Calc. AIT (°C) Type 1	Calc. AIT (°C) Type 2	Calc. AIT (°C) Type 3
N-Phenylacetamide	540	585	559	548
Cycohexaneamine	275	247	228	324
Pyridine	550	526	574	583
2-Nitrobenzeneamine	520	489	498	519
2-Methyl-1-Propanamine	370	344	323	338
2-Methylpyridine	535	532	522	512
Methanamine[b]	430	439	462	400
N,N-Dimethylformamide	440	385	389	504
N,N-Dimethylbenzenamine	370	394	401	362
1,2-Ethanediamine	385	341	320	330
1,1-Dimethylhydrazine	240	353	339	307
Benzenemethanamine	390	455	460	473
2-Methoxybenzenamine[a]	430	441	463	454
Nitromethane	415	407	400	409
N-Butyl-1-butanamine[b]	260	222	223	253
2,6-Diethylbenzenamine	460	424	431	472
Benzenamine	630	518	541	605
N,N-Dimethylbenzenemethanamine	410	344	358	366
3-Chlorobenzenamine	705	678	697	712
Hydrocyanic acid[b]	535	501	524	507
Butanenitrile	500	502	484	434
1-Methyl-2-pyrrolidinone	265	287	294	285
Nitroethane	410	408	416	418
N,N-Diethylbenzenamine	330	331	345	323
2-Methyl-2-propenenitrile[b]	465	520	501	503
4-Chlorobenzenamine	685	679	697	713
N-Phenylbenzenamine[a]	630	645	622	649
2-Hydroxy-2-methylpropanenitrile	540	505	499	496
2-Propenenitrile	480	510	516	499
1-Nitropropane	420	419	437	416
2-Methylbenzenamine	480	501	487	472
Nitrobenzene	480	543	515	498
2-Nitropropane	425	404	425	428
2-Methylpropanenitrile[a]	480	466	455	462
Acetonitrile[a]	525	509	481	494
2-Methyl-2-propanamine	380	405	392	346
N,N-Dipropyl-1-propanamine	180	191	216	223
1-Butanamine	310	376	348	331
3-Methylbenzenamine	480	501	487	458
4-Methylbenzenamine	480	501	488	460

[a]Cross-validation set compound [b]Prediction set compound

Table SM3. Oxygen/Sulfur compounds with their experimental and calculated AIT values.

Compound Name	Exp. AIT (°C)	Calc. AIT (°C) Type 1	Calc. AIT (°C) Type 2	Calc. AIT (°C) Type 3
4-Methylphenol	555	520	560	566
Methoxyethane	190	242	176	237
2-Ethylbutanoic acid	290	423	398	319
1-Phenylethanone[b]	535	498	521	564
2-Pentanone	505	465	484	480
2,4,4-Trimethyl-1-pentanol	395	418	379	394
Propanoic acid ethyl ester	475	415	408	407
1,3-Benzenediol[b]	605	522	560	578
2-Butanone	505	489	509	507
4-Methoxy-4-methyl-2-pentanone	400	417	388	445
4-Heptanol[b]	295	306	288	249
2-Methylpropanal	165	310	198	161
2-Methyl-1-butanol	340	348	335	348
4-Methyl-2-pentanone	475	475	449	459
2-Octanone[a]	420	402	429	421
2,2-Dimethylpropanoic acid	500	557	534	514
1,2-Propanediol	420	379	380	411
1,2-Ethanediol	410	369	375	401
2-Propanol	425	401	416	400
Benzaldehyde[c]	190			
2-Chloropropanoic acid	500	484	458	471
Trimethoxymethane	255	358	250	277
2-Decanone	390	373	383	410
Propanoic acid butyl ester	425	373	384	403
2-Propenoic acid ethyl ester[a]	350	316	329	365
Acetic acid 2-methylpropyl ester	420	426	400	388
2-Methylphenol	555	520	559	571
Acrylic acid[a]	395	393	393	423
2-Nonanone	405	386	413	414
1,2,3-Propanetriol	400	356	347	432
2-Methoxyethanol	285	343	339	346
3-Hydroxy-2-butanone	315	499	314	399
2-Methoxy-2-methylpropane	460	334	459	461
Benzenemethanol	435	441	480	455
2-Methyl-2-butanol[b]	435	459	433	475
1,5-Pentanediol	330	294	283	321
Formic acid methyl ester	450	399	452	487
Methanol	455	414	437	447
2-Methylcyclohexanol	295	306	286	307
Benzoic acid	570	493	534	552
Phenol	595	508	549	550
2,2-Dimethyl-1-propanol	420	455	430	445
2-Propenoic acid butyl ester	275	273	281	352
3-Methyl-2-butanone	475	499	459	476
1,3-Butanediol	375	351	338	347
3-Pentanol	360	351	340	312
Ethanol	400	389	404	382
1-Tetradecanol	240	219	246	227
3-Methyl-1-butanol	340	348	335	348
3-Methylbutanoic acid	385	425	399	364
Acetaldehyde[b]	140	321	154	163
1-Ethoxy-2-propanol	255	356	349	308
2-Pentanol[b]	330	351	340	322
Acetyl chloride[c]	390			
2,5-Hexanedione	490	324	409	442

1,4-Benzenediol	515	520	560	579
2,4-Pentanedione	340	350	426	411
2-Ethoxyethanol	235	319	309	277
2-Butoxyethanol	240	277	272	231
1-Heptanol	275	273	270	266
Cyclohexanol	300	294	277	293
2-Methyl-2-propenoic acid methyl ester[b]	430	354	367	370
3-Pentanone	445	466	483	459
4-Hydroxy-4-methyl-2-pentanone	640	554	648	545
2,6-Dimethyl-4-heptanol	290	328	310	324
Formic acid ethyl ester	440	374	431	468
5-Methyl-2-hexanone	455	451	456	424
2-Propenoic acid 2-methylpropyl ester[a]	350	305	316	352
2-Propenoic acid 2-ethylhexyl ester	245	223	249	288
Methanethiol	360	409	317	365
4-Methylcyclohexanol	295	306	286	295
2-Butanol	390	376	375	352
1-Octadecanol	245	279	260	262
Formic acid 1-methylethyl ester[a]	460	385	424	418
Benzoic acid ethyl ester[a]	490	438	431	536
2,4-Dimethyl-3-pentanol	395	373	357	360
Formic acid	520	459	524	503
2-Propanone	540	512	536	537
1,4-Butanediol	370	316	304	347
Acetic acid[b]	485	485	528	481
3-Hydroxybutanal	245	342	309	246
Furan	390	340	367	409
1-Methoxy-2-propanol	270	356	349	308
Acetic acid pentyl ester	375	375	386	398
Methoxyethene	210	316	224	229
2,3-Butanediol	400	391	384	404
Acetic acid 2-phenylethyl ester	480	478	425	456
2-Ethyl-1-butanol	315	323	303	300
2-Chloroethanol[b]	425	369	376	372
3-Methoxy-3-methyl-1-butanol[b]	395	406	378	399
2-Ethyl-1-hexanol	270	279	265	233
Acetic acid butyl ester	370	394	395	397
Acetic acid ethyl ester[a]	460	438	431	411
1-Decanol	250	230	251	221
2-Methyl-1-propanol	430	401	416	400
1-Dodecanol	250	216	246	220
Tetrahydrofuran[b]	230	190	269	257
2-Hydroxybenzoic acid methyl ester	450	470	446	446
2-Propenoic acid methyl ester	415	340	359	375
1-Propanol	405	364	366	362
Propanoic acid ethenyl ester	385	406	398	411
Butanoic acid	440	437	430	403
Pentanoic acid[a]	375	414	408	392
Octadecanoic acid	395	411	385	405
2-Methylpropanoic acid	500	472	453	470
Nonanoic acid	405	346	369	396
Hexanoic acid	380	393	395	387
2-Octanol	265	289	272	238
1,1-Dioxyethane	230	212	268	227
2-Methyl-2-propanol[b]	470	485	486	489
Acetic acid ethenyl ester	385	428	423	387
4-Methyl-2-pentanol	335	360	346	355
1,4-Dioxane	375	171	291	343
Propanoic acid pentyl ester[b]	375	356	376	404
2-Methyl-2-propenoic acid	385	404	395	428

Pentanal	210	250	192	218
1-Hexadecanol	245	239	249	241
Acetic acid propyl ester[a]	430	415	409	399
2-Chloro-1,1-dimethoxyethane	230	245	297	190
Ethanethiol	295	387	343	265
2-Hydroxypropanoic acid methyl ester[a]	400	392	335	417
2-Methylbutanoic acid[b]	420	448	418	378
1-Pentanol	300	315	303	323
2-Ethoxy-1-propanol[b]	255	328	312	254
2-Propen-1-ol[a]	375	354	330	371
Acetic acid methyl ester	475	462	471	435
Acetic acid anhydride	330	445	415	350
2-Methyl-2-pentanol	415	435	401	426
Butanal	190	273	182	198
4-Methyl-3-penten-2-one	340	358	353	363
1-Octanol[a]	270	256	261	242
2-Propyn-1-ol	365	399	418	373
Formic acid propyl ester	450	350	417	445
Propanoic acid	485	461	469	431
2,5-Furandione[c]	380			
Ethoxyethene	200	291	236	189
7-Ethyl-2-methyl-4-undecanol	250	249	248	210
Propanal	190	298	171	179
1-Hexanol	290	293	283	294
2-Methylpentanal	195	262	204	187
Cyclohexanone	430	411	439	427
Acetic acid cyclohexyl ester	330	345	368	343
Methoxybenzene[a]	475	396	456	432
2-Methoxy-2-methylbutane	345	309	327	329
Dimethoxymethane	235	238	232	269
2-Methyl-2,4-pentanediol	425	445	396	416
2-Methyl-2-propenoic acid butyl ester	290	291	300	279
1-Nonanol	260	241	255	229
1-Butanol	340	339	331	345
Formic acid 2-methylpropyl ester	320	361	408	404

[a]Cross-validation set compound [b]Prediction set compound [c]Outlier compound

Table SM4. Alcohol/Ether compounds with their experimental and calculated AIT values.

Compound Name	Exp. AIT (°C)	Calc. AIT (°C) Type 1	Calc. AIT (°C) Type 2	Calc. AIT (°C) Type 3
4-Methylphenol	555	536	543	546
Methoxyethane[a]	190	229	227	237
2,4,4-Trimethyl-1-pentanol	395	371	384	404
1,3-Benzenediol[b]	605	552	557	570
4-Heptanol[b]	295	271	264	294
2-Methyl-1-butanol	340	362	370	353
1,2-Propanediol	420	402	396	403
1,2-Ethanediol	410	354	369	409
2-Propanol	425	407	418	407
Trimethoxymethane	255	239	234	237
2-Methylphenol	555	530	539	546
1,2,3-Propanetriol	400	424	423	417
2-Methoxyethanol	285	284	290	274
2-Methoxy-2-methylpropane	460	410	391	412
Benzenemethanol	435	479	499	447
2-Methyl-2-butanol[b]	435	480	432	432
1,5-Pentanediol	330	328	347	316
Methanol	455	456	424	434
2-Methylcyclohexanol	295	337	307	302
Phenol	595	500	515	542
2,2-Dimethyl-1-propanol	420	478	434	432
1,3-Butanediol	375	375	376	373
3-Pentanol	360	341	344	357
Ethanol	400	391	390	412
1-Tetradecanol	240	231	232	230
3-Methyl-1-butanol	340	362	370	353
1-Ethoxy-2-propanol[a]	255	285	287	268
2-Pentanol[b]	330	327	331	353
1,4-Benzenediol	515	564	559	571
2-Ethoxyethanol	235	246	248	256
2-Butoxyethanol	240	232	235	239
1-Heptanol[a]	275	262	262	273
Cyclohexanol	300	319	284	294
2,6-Dimethyl-4-heptanol	290	335	334	292
4-Methylcyclohexanol	295	346	322	300
2-Butanol[a]	390	403	405	384
1-Octadecanol	245	240	233	229
2,4-Dimethyl-3-pentanol	395	357	359	354
1,4-Butanediol	370	340	350	348
Furan	390	366	409	412
1-Methoxy-2-propanol	270	285	287	268
Methoxyethene	210	241	240	236
2,3-Butanediol	400	446	405	404
2-Ethyl-1-butanol	315	309	308	323
2-Chloroethanol[a]	425	431	433	406
3-Methoxy-3-methyl-1-butanol	395	363	367	394
2-Ethyl-1-hexanol	270	268	259	270
1-Decanol	250	237	239	239
2-Methyl-1-propanol	430	407	417	407
1-Dodecanol	250	232	234	232
Tetrahydrofuran[b]	230	257	275	237
1-Propanol	405	368	379	390
2-Octanol	265	296	296	269
1,1-Diethoxyethane	230	280	282	233
2-Methyl-2-propanol[b]	470	472	451	439

4-Methyl-2-pentanol	335	332	336	352
1,4-Dioxane	375	305	322	364
1-Hexadecanol[a]	245	234	231	229
2-Chloro-1,1-dimethoxyethane	230	264	271	234
1-Pentanol	300	298	300	328
2-Ethoxy-1-propanol[b]	255	271	269	253
2-Propen-1-ol	375	378	389	387
2-Methyl-2-pentanol	415	375	386	419
1-Octanol	270	251	251	257
2-Propyn-1-ol	365	444	446	387
Ethoxyethene	200	228	230	233
7-Ethyl-2-methyl-4-undecanol	250	293	249	234
1-Hexanol	290	277	277	297
Methoxybenzene	475	378	415	465
2-Methoxy-2-methylbutane	345	416	405	394
Dimethoxymethane	235	230	229	236
2-Methyl-2,4-pentanediol	425	416	453	432
1-Nonanol	260	243	244	246
1-Butanol[a]	340	331	338	360

[a]Cross-validation set compound [b]Prediction set compound

Table SM5. Correlation matrices for the descriptors in the low-temperature hydrocarbon models.

Type 1 Model					
	PNSA 2	NBR	V6P	WTPT 2	dHoF
PNSA 2	1.000				
NBR	0.264	1.000			
V6P	0.181	-0.413	1.000		
WTPT 2	0.096	0.656	-0.719	1.000	
dHoF	-0.262	0.148	0.518	-0.484	1.000

Type 3 Model					
	PNSA 2	DPSA 3	V2	N4P	1SP2
PNSA 2	1.000				
DPSA 3	-0.769	1.000			
V2	-0.115	0.510	1.000		
N4P	-0.016	0.229	0.753	1.000	
1SP2	-0.640	0.350	-0.309	-0.203	1.000

Table SM6. Correlation matrices for the descriptors in the high-temperature hydrocarbon models.

Type 1 Model						
	NSB	NBR	MOLC 8	N4PC	V5PC	1SP3
NSB	1.000					
NBR	-0.462	1.000				
MOLC 8	0.696	-0.388	1.000			
N4PC	0.482	0.155	0.800	1.000		
V5PC	0.778	-0.170	0.700	0.719	1.000	
1SP3	0.834	-0.689	0.759	0.458	0.691	1.000

Type 3 Model						
	QNEG	FPSA 2	NAB	N4PC	ALLP 4	1SP3
QNEG	1.000					
FPSA 2	-0.362	1.000				
NAB	0.448	-0.222	1.000			
N4PC	0.018	0.618	0.193	1.000		
ALLP 4	0.508	0.195	0.711	0.521	1.000	
1SP3	-0.485	0.828	-0.551	0.458	-0.171	1.000

Table SM7. Correlation matrices for the descriptors in the nitrogen compound models.

Type 1 Model						
	QPOS	WNSA 1	NC	NSB	1SP3	2SP3
QPOS	1.000					
WNSA 1	0.279	1.000				
NC	-0.468	0.493	1.000			
NSB	-0.084	-0.331	0.209	1.000		
1SP3	-0.029	-0.344	0.059	0.467	1.000	
2SP3	-0.133	-0.385	0.123	0.716	0.133	1.000

Type 3 Model						
	DPOL	PNSA 1	DPSA 1	WNSA 1	WNSA 3	RDTA
DPOL	1.000					
PNSA 1	0.506	1.000				
DPSA 1	-0.707	-0.812	1.000			
WNSA 1	0.272	0.937	-0.576	1.000		
WNSA 3	-0.877	-0.673	0.732	-0.498	1.000	
RDTA	-0.571	-0.172	0.217	-0.071	0.449	1.000

Table SM8. Correlation matrices for the descriptors in the oxygen/sulfur compound models.

Type 1 Model							
	QPOS	QNEG	NSB	NDB	N3C	KETO	MOMH 1
QPOS	1.000						
QNEG	-0.864	1.000					
NSB	0.178	-0.227	1.000				
NDB	0.042	0.220	-0.161	1.000			
N3C	0.109	-0.074	0.107	0.108	1.000		
KETO	-0.139	0.109	-0.016	0.221	0.115	1.000	
MOMH 1	0.141	-0.142	0.805	-0.079	-0.118	-0.046	1.000

Type 3 Model							
	QNEG	FNSA 2	MOLC 7	N2P	ALDE	MOMH 7	dHoF
QNEG	1.000						
FNSA 2	0.113	1.000					
MOLC 7	-0.105	0.027	1.000				
N2P	-0.175	-0.230	0.316	1.000			
ALDE	0.078	0.068	-0.068	-0.170	1.000		
MOMH 7	-0.234	-0.001	0.091	0.872	-0.104	1.000	
dHoF	0.293	0.210	-0.098	-0.432	0.145	-0.558	1.000

Table SM9. Correlation matrices for the descriptors in the alcohol/ether compound models.

Type 1 Model						
	QPOS	RPCG	SAAA	RDTA	V4P	N2P
QPOS	1.000					
RPCG	0.611	1.000				
SAAA	0.750	0.454	1.000			
RDTA	0.924	0.534	0.666	1.000		
V4P	0.227	-0.425	-0.061	0.276	1.000	
N2P	0.153	-0.520	-0.069	0.188	0.880	1.000

Type 3 Model						
	RDTA	MOLC 1	N2P	N3C	WTPT 3	MOMH 7
RDTA	1.000					
MOLC 1	0.197	1.000				
N2P	0.188	0.849	1.000			
N3C	0.044	0.036	0.429	1.000		
WTPT 3	-0.416	-0.100	-0.160	-0.053	1.000	
MOMH 7	0.235	0.895	0.862	0.091	-0.128	1.000

Supporting Material Figure Captions

Figure SM1. Calculated versus observed AIT values for the training set and cross-validation set from the Type 3 high-temperature hydrocarbon model.

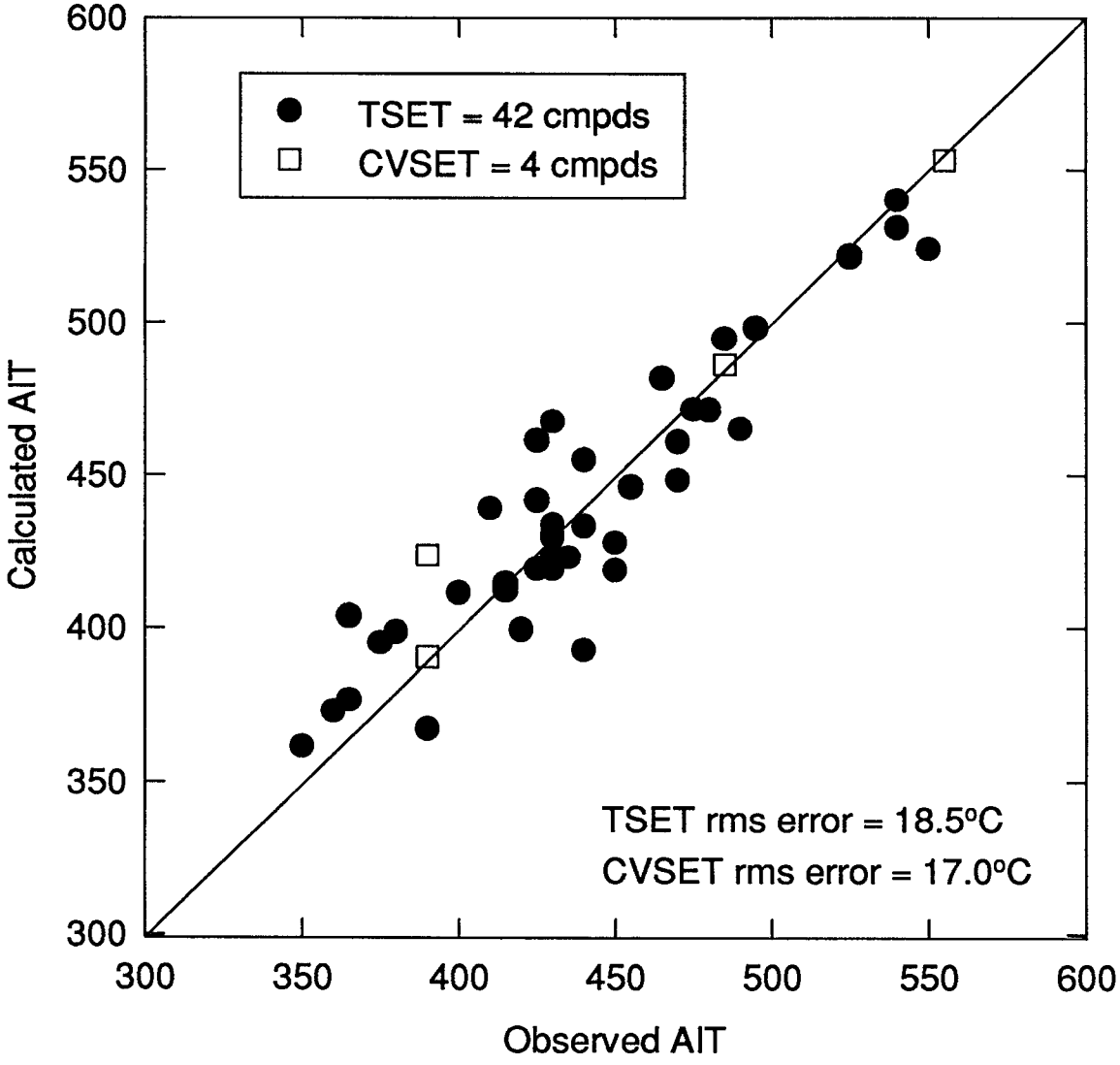
Figure SM2. Validation of the Type 3 high-temperature hydrocarbon model using the external prediction set.

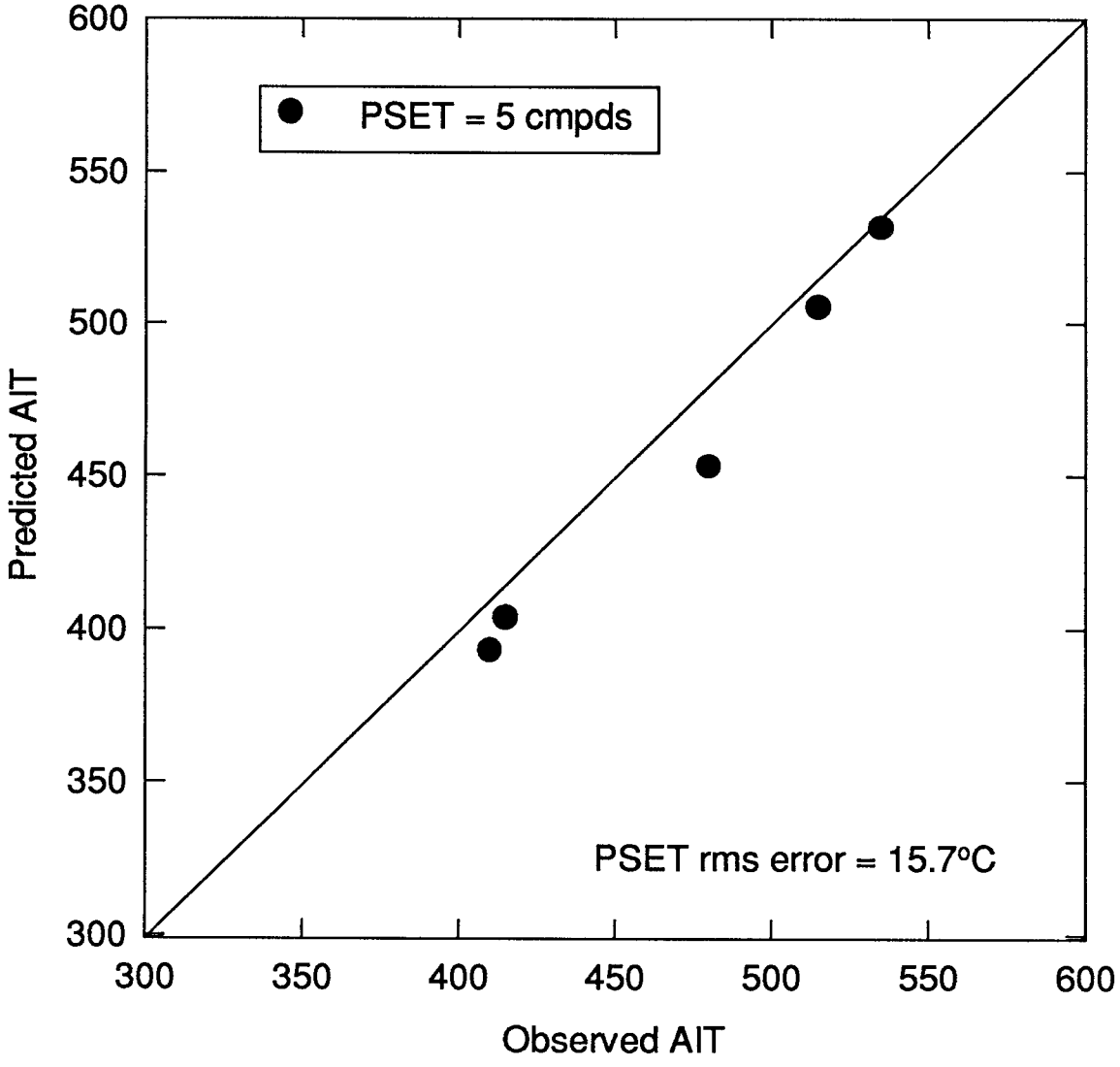
Figure SM3. Calculated versus observed AIT values for the training set and cross-validation set from the Type 3 oxygen/sulfur compound model.

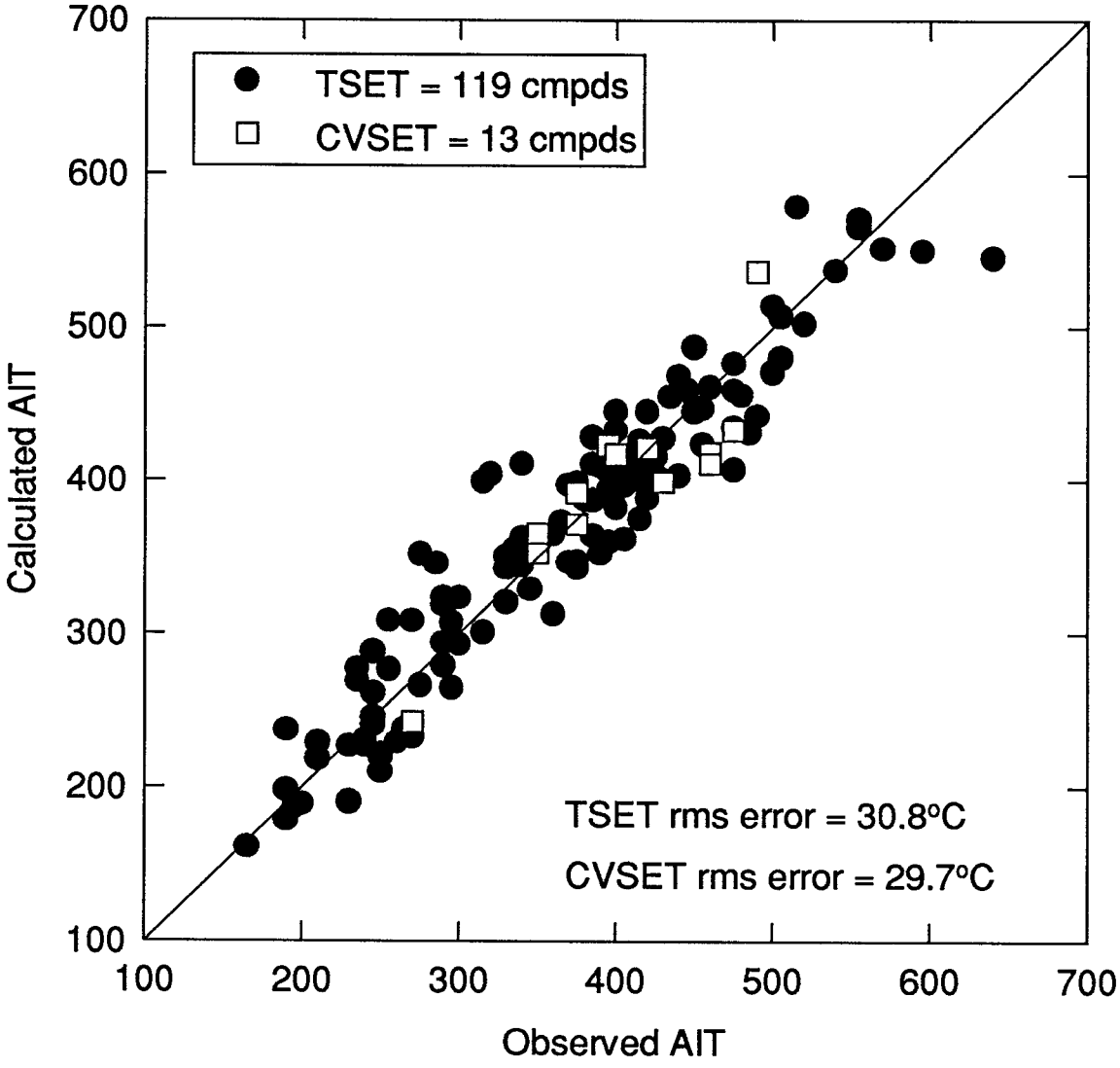
Figure SM4. Validation of the Type 3 oxygen/sulfur compound model using the external prediction set.

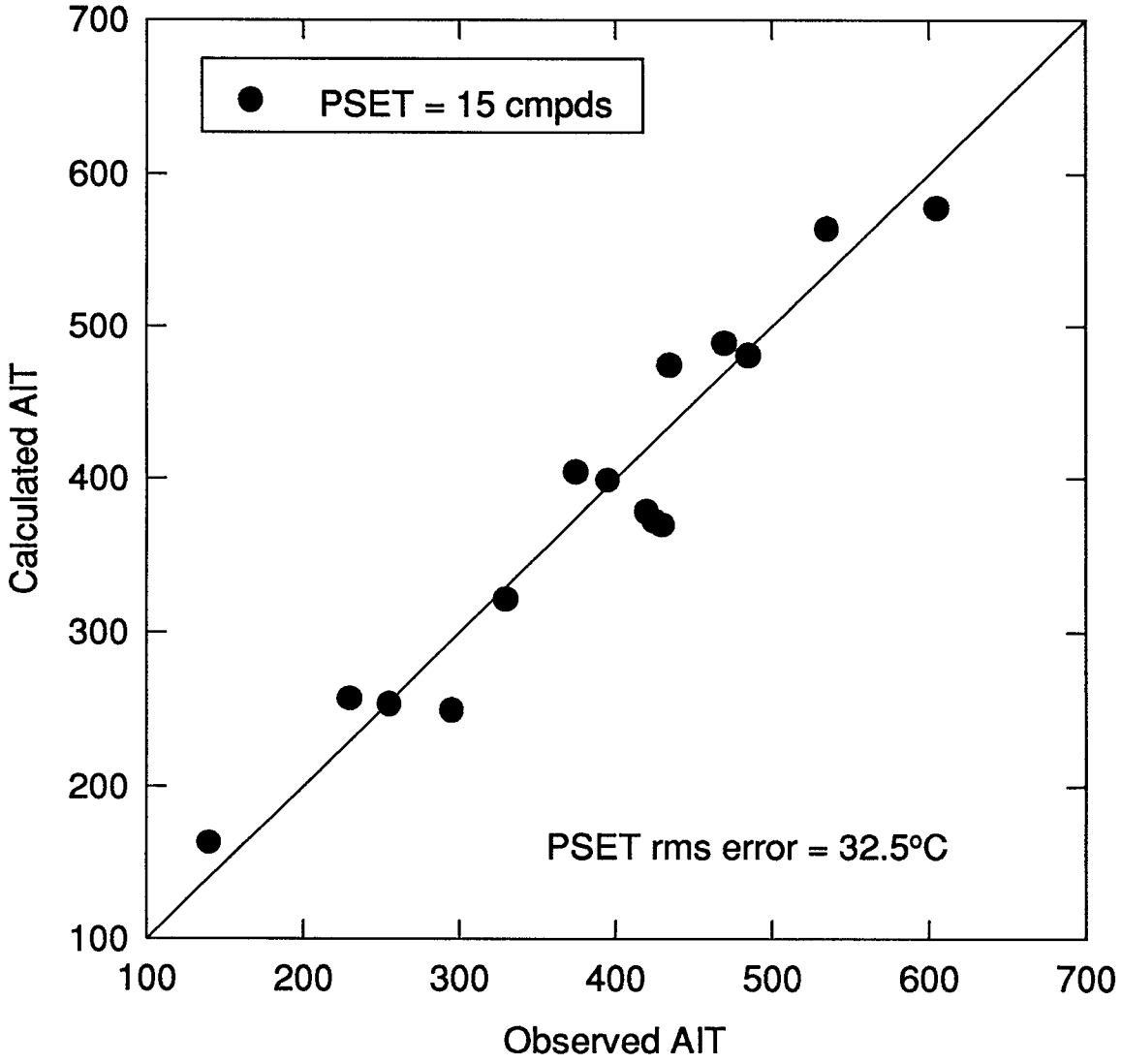
Figure SM5. Calculated versus observed AIT values for the training set and cross-validation set from the Type 3 alcohol/ether compound model.

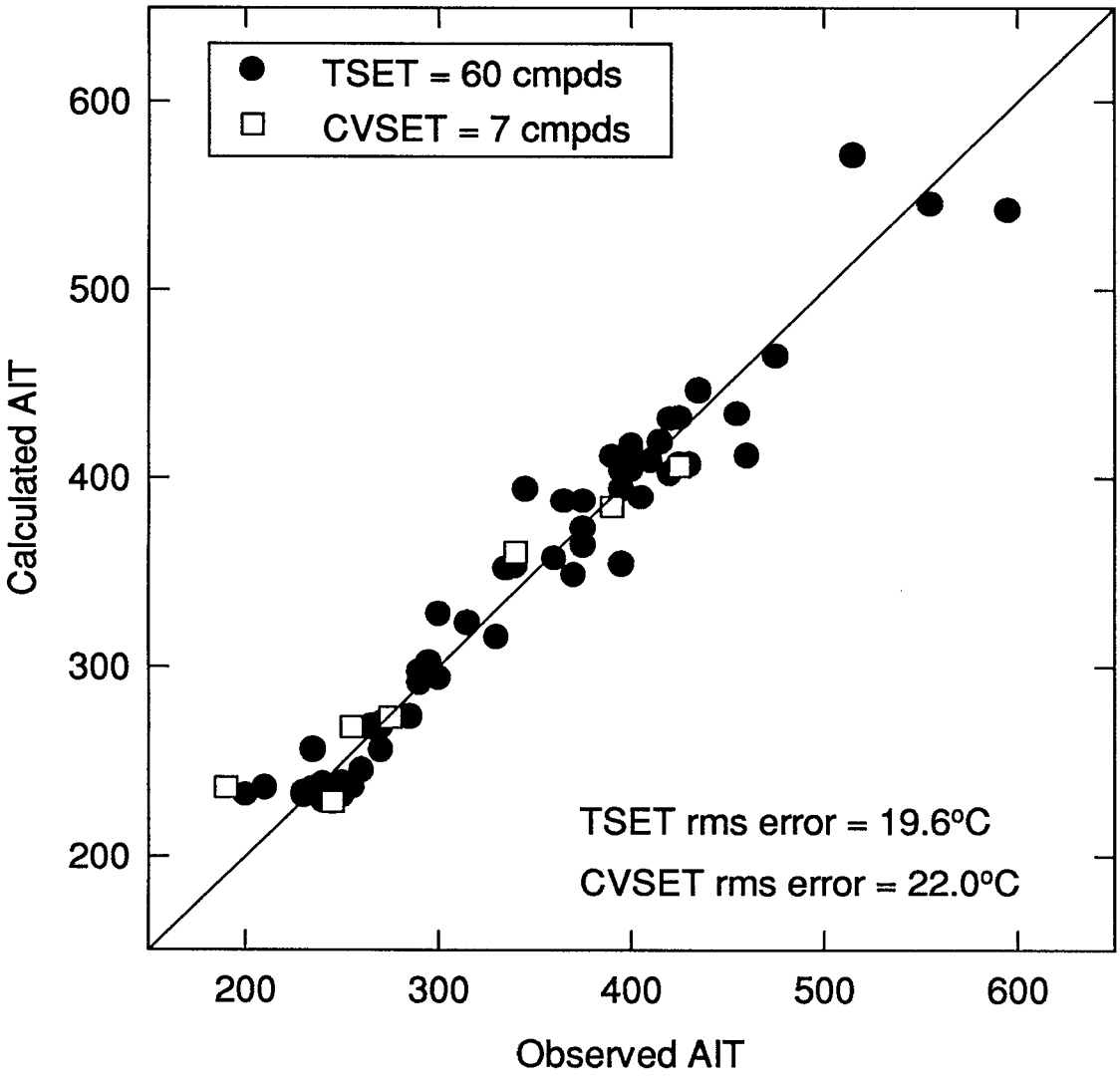
Figure SM6. Validation of the Type 3 alcohol/ether compound model using the external prediction set.

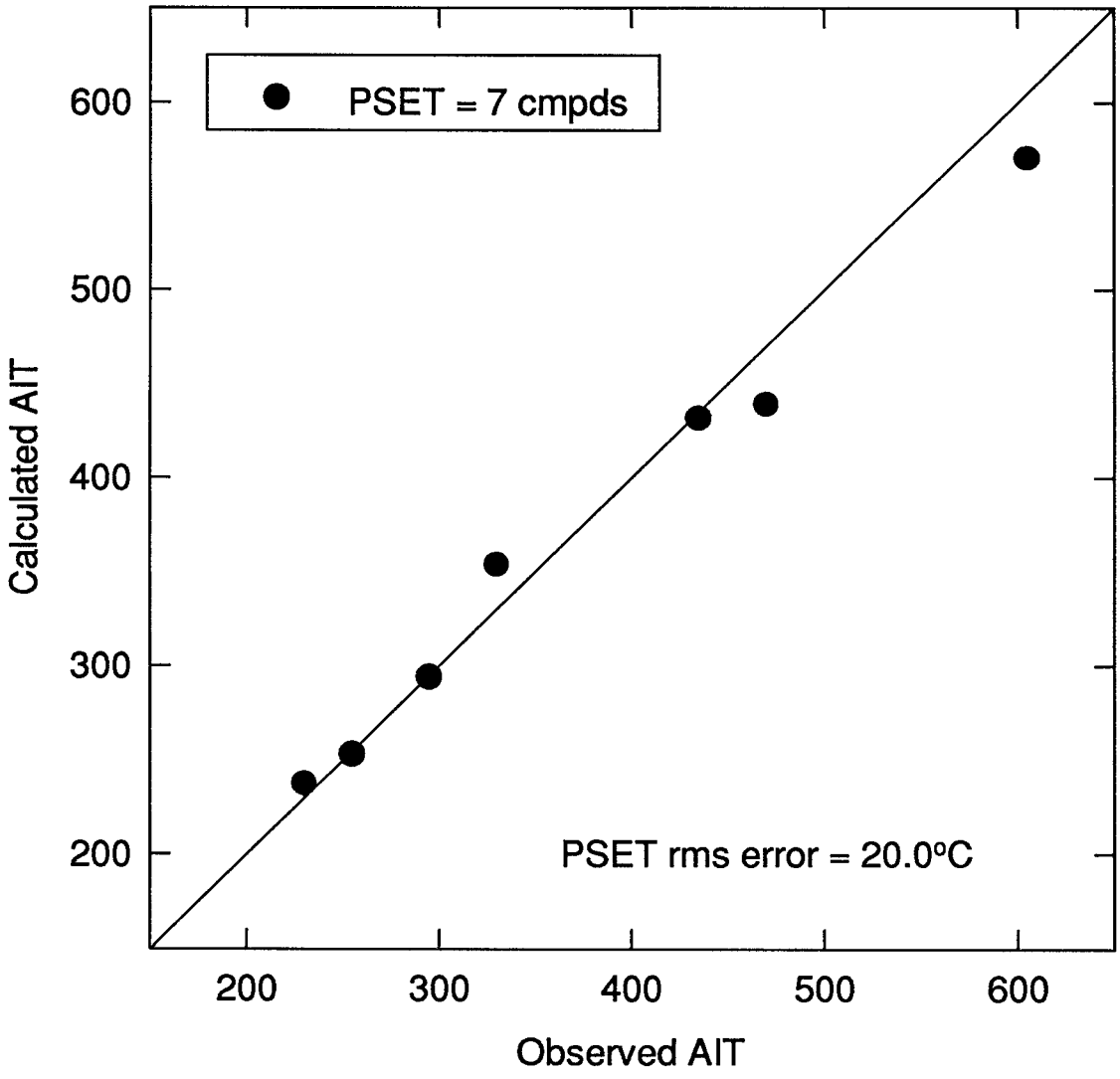

TSET = 42 cmpds
CVSET = 4 cmpds
TSET rms error = 18.5°C
CVSET rms error = 17.0°C
Calculated AIT
Observed AIT
300
350
400
450
500
550
600


PSET = 5 cmpds
PSET rms error = 15.7°C
Predicted AIT
Observed AIT
600
550
500
450
400
350
300
300
350
400
450
500
550
600


TSET = 119 cmpds
CVSET = 13 cmpds
TSET rms error = 30.8°C
CVSET rms error = 29.7°C
Calculated AIT
Observed AIT
100
200
300
400
500
600
700


PSET = 15 cmpds
PSET rms error = 32.5°C
Calculated AIT
Observed AIT
100
200
300
400
500
600
700


TSET = 60 cmpds
CVSET = 7 cmpds
TSET rms error = 19.6°C
CVSET rms error = 22.0°C
Calculated AIT
Observed AIT
200
300
400
500
600


PSET = 7 cmpds
PSET rms error = 20.0°C
Calculated AIT
Observed AIT
200
300
400
500
600