

Table 1: Supporting information

	%AAD Vapor pressures				%AAD liquid densities			
	NP	T range (K)	without neighborhood-correction	with neighborhood-correction	NP	T range (K)	without neighborhood-correction	with neighborhood-correction
n-butane	11	140-420	12.6	12.6	11	311-394	2.4	2.4
n-pentane	11	223-470	11.2	11.2	11	143-443	1.5	1.5
n-hexane	11	196-503	10.9	10.9	11	193-478	1.1	1.1
n-heptane	11	194-540	7.9	7.9	11	183-513	0.9	0.9
n-octane	11	228-569	7.6	7.6	11	333-533	0.7	0.7
n-nonane	11	311-511	6.6	6.6	11	223-533	0.5	0.5
n-decane	11	268-490	3.2	3.2	11	244-583	0.6	0.6
n-undecane	11	348-499	3.6	3.6	11	253-573	1.0	1.0
n-dodecane	11	289-520	2.5	2.5	11	263-623	1.6	1.6
n-tridecane	11	290-540	2.4	2.4	11	273-573	1.2	1.2
n-tetradecane	11	280-559	1.7	1.7	11	283-523	1.1	1.1
n-pentadecane	11	346-577	1.4	1.4	11	283-543	1.4	1.4
n-hexadecane	11	295-594	1.2	1.2	11	291-563	1.7	1.7
n-heptadecane	11	390-609	3.0	3.0	11	295-613	0.9	0.9
n-octadecane	11	318-624	2.3	2.3	11	302-593	2.3	2.3
n-nonadecane	11	306-638	2.8	2.8	11	305-603	2.5	2.5
n-eicosane	11	344-652	3.8	3.8	11	310-613	2.4	2.4
n-henicosane	11	318-630	3.7	3.7	11	314-372	0.3	0.3
n-docosane	11	318-668	1.3	1.3	11	318-373	0.3	0.3
n-tricosane	11	418-693	4.0	4.0	11	321-372	0.3	0.3
n-tetracosane	11	379-588	4.1	4.1	11	343-343	0.2	0.2
n-pentacosane	11	379-674	3.0	3.0	11	293-373	0.5	0.5
n-hexacosane	11	379-684	4.3	4.3	11	330-431	0.7	0.7
n-heptacosane	11	351-543	11.1	11.1	11	333-372	0.2	0.2
n-octacosane	11	418-588	3.9	3.9	11	335-573	2.4	2.4
n-nonacosane	11	456-714	0.3	0.3	11	343-343	0.3	0.3

n-triacontane	11	463-722	1.3	1.3	11	343-363	0.2	0.2
n-dotriacontane	11	475-739	4.1	4.1	11	348-373	0.2	0.2
n-hexatriacontane	11	497-769	8.7	8.7	11	353-573	2.7	2.7
mean alkanes			4.6	4.6			1.1	1.1
2-methylpropane	11	239-407	2.2	2.2	11	213-378	9.1	9.1
2-methyl-butane	11	217-448	6.3	6.3	11	150-433	6.4	6.4
2-methylpentane	11	241-498	2.1	2.1	11	258-333	5.3	5.3
3-methylpentane	11	243-504	7.7	7.7	11	266-339	3.7	3.7
2-methylhexane	11	271-530	0.6	0.6	11	272-503	5.7	5.7
3-methylhexane	11	272-535	1.5	1.5	11	233-503	3.2	3.2
2-methylheptane	11	222-560	1.8	1.8	11	263-523	4.4	4.4
3-methylheptane	11	223-564	1.0	1.0	11	263-533	3.5	3.5
4-methylheptane	11	293-562	2.8	2.8	11	263-533	3.5	3.5
3-methyloctane	11	306-445	0.9	0.9	11	283-313	3.2	3.2
4-methyloctane	11	305-443	6.1	6.1	11	283-313	3.3	3.3
2-methylnonane	11	325-469	2.8	2.8	11	273-313	3.8	3.8
3-methylnonane	11	325-470	0.8	0.8	11	273-313	3.0	3.0
mean methyls			2.8	2.8			4.5	4.5
2,2-dimethylpropane	11	258-434	26.6	4.5	11	253-403	4.0	4.6
2,2-dimethylbutane	11	199-489	8.7	4.7	11	269-320	6.8	6.3
2,2-dimethylpentane	11	261-513	11.5	0.7	11	150-493	5.3	5.4
3,3-dimethylpentane	11	213-536	4.9	3.7	11	272-503	8.1	6.7
2,2-dimethylhexane	11	272-513	11.6	1.3	11	276-550	4.9	5.2
3,3-dimethylhexane	11	279-562	2.7	0.8	11	272-533	10.2	9.3
2,2-dimethylheptane	11	303-433	11.7	2.7	11	293-298	3.6	3.7
2,2-dimethyloctane	11	316-458	9.4	1.2	11	293-298	3.2	3.3
mean dimethyls with >C<			10.9	2.4			6.5	6.1
2,3-dimethylbutane	11	238-500	12.1	12.1	11	266-473	11.4	11.4
2,3-dimethylpentane	11	205-523	9.2	9.2	11	272-503	8.1	8.1
2,4-dimethylpentane	11	262-520	8.2	8.2	11	272-493	10.6	10.6
2,3-dimethylhexane	11	283-563	2.5	2.5	11	272-533	7.9	7.9
2,4-dimethylhexane	11	278-553	9.2	9.2	11	272-523	9.5	9.5

2,5-dimethylhexane	11	278-550	10.2	10.2	11	255-513	9.4	9.4
3,4-dimethylhexane	11	272-533	5.1	5.1	11	284-569	6.7	6.7
2,6-dimethylheptane	11	299-435	6.1	6.1	11	286-360	8.1	8.1
2,3-dimethyloctane	11	321-466	4.5	4.5	11	293-298	6.1	6.1
2,4-dimethyloctane	11	316-457	8.3	8.3	11	281-298	7.1	7.1
2,5-dimethyloctane	11	317-460	4.2	4.2	11	293-298	6.6	6.6
2,6-dimethyloctane	11	319-462	5.7	5.7	11	293-298	7.0	7.0
2,7-dimethyloctane	11	271-461	7.6	7.6	11	273-393	7.3	7.3
mean dimethyls with no >C<			7.2	7.2			8.1	8.1
2,2,3-trimethylbutane	11	254-528	3.3	3.8	11	261-503	2.5	1.4
2,2,3-trimethylpentane	11	284-564	2.8	1.7	11	272-533	3.9	3.2
2,2,4-trimethylpentane	11	199-544	9.1	12.4	11	166-513	1.1	1.1
2,3,3-trimethylpentane	11	280-573	9.8	3.8	11	272-543	5.6	3.3
2,2,5-trimethylhexane	11	206-424	14.8	10.7	11	283-523	0.4	0.6
2,4,4-trimethylhexane	11	300-432	5.6	4.5	11	283-323	2.0	1.5
3,3,5-trimethylheptane	11	313-458	4.0	4.2	11	293-298	2.3	2.0
mean trimethyls with 1 >C<			7.1	5.9			2.6	1.9
2,2,3,3-tetramethylbutane	11	375-406	5.4	5.8	11	374-510	16.8	12.5
2,2,3,3-tetramethylpentane	11	307-442	20.0	7.2	11	288-323	14.7	12.8
2,2,3,4-tetramethylpentane	11	301-434	3.8	4.1	11	288-298	1.0	1.5
2,2,4,4-tetramethylpentane	11	293-423	2.4	10.8	11	288-303	10.5	9.5
2,3,3,4-tetramethylpentane	11	308-443	16.3	1.9	11	283-323	0.9	0.2
2,2,3,3-tetramethylhexane	11	314-463	3.3	6.0	11	293-298	12.4	11.1
2,2,5,5-tetramethylhexane	11	300-438	20.6	11.8	11	293-298	7.2	6.7
2,2,4,4,6,8,8-heptamethylnonane	11	424-545	6.1	7.6	11	298-313	6.6	5.8
2,6,10,15,19,23-hexamethyltetracosane	11	468-536	22.6	22.6	11	273-562	7.1	7.1
mean multimethyls			11.2	8.7			8.6	7.5
3-ethylpentane	11	266-541	2.8	2.8	11	155-513	3.2	3.2
3-ethylhexane	11	286-565	4.7	4.7	11	272-533	1.8	1.8
3-ethylheptane	11	305-384	9.8	9.8	11	293-298	2.5	2.5
3-ethyl-2-methylpentane	11	283-560	3.3	3.3	11	261-533	6.1	6.1
2,2-dimethyl-3-ethylpentane	11	296-435	12.0	12.0	11	293-298	2.5	2.3

2,4-dimethyl-3-ethylpentane	11	298-438	12.9	12.9	11	293-298	9.3	9.3
2,3,4-trimethylpentane	11	223-566	6.1	6.0	11	272-533	12.0	12.0
3,3-diethylpentane	11	304-448	12.6	5.6	11	288-298	9.5	8.3
3-ethyl-3-methylpentane	11	249-576	10.0	2.9	11	273-323	9.0	8.0
others			8.2	6.7			6.2	5.9

Table 2: Supporting information

	heterosegmented GC-PC-SAFT with neighborhood correction	Marrero et Gani [1] (MG)	Constantino u [2] (Const)	Experimental (Exp)[1]	% AAD heterosegmented GC-PC-SAFT with neighborhood correction / Exp	% AAD MG/ Exp	% AAD CONST/ Exp
	T <sub>b</sub> (K)	T <sub>b</sub> (K)	T <sub>b</sub> (K)	T <sub>b</sub> (K)			
n-butane	275.5	253.7	263.1	272.65	1.0	7.0	3.5
n-pentane	312.1	299.5	309.5	309.2	0.9	3.1	0.1
n-hexane	345.0	337.4	347.2	341.9	0.9	1.3	1.6
n-heptane	374.7	369.8	379.1	371.6	0.8	0.5	2.0
n-octane	401.8	398.1	406.6	398.9	0.7	0.2	1.9
n-nonane	426.7	423.2	430.9	424.0	0.6	0.2	1.6
n-decane	449.8	445.7	452.6	447.3	0.6	0.3	1.2
n-undecane	471.2	466.2	472.2	469.1	0.5	0.6	0.7
n-dodecane	491.3	485.0	490.1	489.5	0.4	0.9	0.1
n-tridecane	510.1	502.3	506.6	508.6	0.3	1.2	0.4
n-tetradecane	527.8	518.3	521.8	526.7	0.2	1.6	0.9
n-pentadecane	544.6	533.3	535.9	543.8	0.1	1.9	1.5
n-hexadecane	560.5	547.3	549.2	560.0	0.1	2.3	1.9
n-heptadecane	575.6	560.5	561.6	575.3	0.0	2.6	2.4
n-octadecane	590.0	572.9	573.4	589.9	0.0	2.9	2.8
n-nonadecane	603.7	584.7	584.5	603.1	0.1	3.1	3.1
n-eicosane	616.8	595.9	595	616.9	0.0	3.4	3.6
n-henicosane	629.4	606.6	605	629.7	0.0	3.7	3.9
n-docosane	641.5	616.7	614.5	641.8	0.1	3.9	4.3
n-tricosane	653.1	626.5	623.6	653.4	0.0	4.1	4.6
n-tetracosane	664.2	635.8	632.4	664.5	0.0	4.3	4.8
n-pentacosane	675.0	644.7	640.7	675.1	0.0	4.5	5.1
n-hexacosane	685.4	653.3	648.8	685.4	0.0	4.7	5.3

n-heptacosane	695.4	661.6	656.5	685.3	1.5	3.5	4.2
n-octacosane	705.1	669.6	664	704.8	0.0	5.0	5.8
n-nonacosane	714.5	677.3	671.1	714.0	0.1	5.1	6.0
n-triacontane	723.6	684.8	678.1	722.9	0.1	5.3	6.2
n-dotriacontane	740.9	699.0	691.3	738.9	0.3	5.4	6.4
n-hexatriacontane	772.7	724.9	715.4	770.2	0.3	5.9	7.1
mean alkanes					0.3	3.1	3.2
2-methylpropane	260.2	232.3	219.3	261.4	0.5	11.1	16.1
2-methyl-butane	299.1	282.2	287.3	301.0	0.6	6.2	4.6
2-methylpentane	332.7	322.9	328.9	333.4	0.2	3.1	1.3
3-methylpentane	334.0	322.9	333.6	336.4	0.7	4.0	0.8
2-methylhexane	362.9	357.4	363.5	363.2	0.1	1.6	0.1
3-methylhexane	364.3	357.4	367.5	365.0	0.2	2.1	0.7
2-methylheptane	390.5	387.2	393.1	390.8	0.1	0.9	0.6
3-methylheptane	391.9	387.2	396.5	392.1	0.0	1.2	1.1
3-methyloctane	417.2	413.5	422	417.4	0.0	0.9	1.1
2-methylnonane	439.1	437.0	441.9	440.2	0.3	0.7	0.4
3-methylnonane	440.6	437.0	444.6	441.0	0.1	0.9	0.8
mean methyls					0.3	3.0	2.5
2,2-dimethylbutane	322.2	311.3	317.1	322.9	0.2	3.6	1.8
2,2-dimethylpentane	352.5	347.4	353.6	352.3	0.1	1.4	0.4
3,3-dimethylpentane	357.6	347.1	355.3	359.2	0.4	3.4	1.1
2,2-dimethylhexane	380.3	378.5	384.5	380.0	0.1	0.4	1.2
3,3-dimethylhexane	385.1	378.2	386	385.1	0.0	1.8	0.2
2,2-dimethylheptane	406.0	405.8	411.4	405.8	0.1	0.0	1.4
2,2-dimethyloctane	429.7	430.1	435.1	430.1	0.1	0.0	1.2
mean dimethyls with >C<					0.1	1.5	1.0
2,3-dimethylbutane	327.7	324.1	339	333.1	1.6	2.7	1.8
2,3-dimethylpentane	360.2	358.5	357.5	362.9	0.7	1.2	1.5

2,4-dimethylpentane	351.9	347.8	351	353.6	0.5	1.6	0.7
2,3-dimethylhexane	388.4	388.2	387.9	388.8	0.1	0.2	0.2
2,4-dimethylhexane	381.3	375.5	382.3	382.6	0.3	1.9	0.1
2,5-dimethylhexane	379.9	375.4	378.6	382.3	0.6	1.8	1.0
3,4-dimethylhexane	389.8	388.3	391.4	390.9	0.3	0.7	0.1
2,6-dimethylheptane	405.5	403.0	406.2	408.4	0.7	1.3	0.5
2,3-dimethyloctane	437.8	437.8	437.8	437.5	0.1	0.1	0.1
2,4-dimethyloctane	430.5	427.7	433.4	429.1	0.3	0.3	1.0
2,7-dimethyloctane	429.1	427.6	430.6	433.0	0.9	1.2	0.6
mean dimethyls with no >C<					0.6	1.2	0.7
2,2,3-trimethylbutane	352.6	333.6	335.9	354.0	0.4	5.8	5.1
2,2,3-trimethylpentane	382.4	379.7	373.3	383.0	0.2	0.9	2.5
2,2,4-trimethylpentane	372.3	366.4	369.4	372.4	0.0	1.6	0.8
2,3,3-trimethylpentane	386.4	384.7	391.2	387.9	0.4	0.8	0.9
2,2,5-trimethylhexane	397.6	395.1	398.2	397.2	0.1	0.5	0.2
2,4,4-trimethylhexane	403.1	394.8	399.6	403.8	0.2	2.2	1
mean trimethyls with 1 >C<					0.2	2.0	1.8
2,2,3,3-tetramethylbutane	412.3	403.5	431.0	413.4	0.3	2.4	4.3
2,2,3,3-tetramethylpentane	408.8	399.3	403.6	406.2	0.7	1.7	0.6
2,2,3,4-tetramethylpentane	391.0	386.9	389.8	395.4	1.1	2.2	1.4
2,2,4,4-tetramethylpentane	415.0	416.7	407.7	414.7	0.1	0.5	1.7
2,3,3,4-tetramethylpentane	435.9	428.0	452.7	433.5	0.6	1.3	4.4
2,2,3,3-tetramethylhexane	414.0	413.2	416.1	410.6	0.8	0.6	1.3
mean multimethyls					0.6	1.5	2.3