Supporting Information

Assessment of low Global Warming Potential Refrigerants for drop-in Replacement by Connecting their Molecular Features to their Performance

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Number of figures: 8 (Figures S1-S8)

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Table S1. Environmental, and Safety for refrigerants examined in this work included in **Table 1**.[1–8]

Substance	GWP	ODP	Toxicity	Flammability
R41	116	0	A	2
R32	677	0	A	2L
R23	12400	0	A	1
R161	4	0	A	2
R152a	138	0	A	2
R134a	1300	0	A	1
R125	3170	0	A	1
R245fa	858	0	B	1
R236fa	8060	0	A	1
R227ea	3350	0	A	1
R1123	3	0	A	1
R1243zf	1	0	A	2
R1234yf	0	0	A	2L
R1234ze(E)	1	0	A	2L
R1225ye(Z)	3	0	A	1
R1336mzz(Z)	2	0	A	1
R1233zd(E)	5	0.00024	A	1
R1224yd(Z)	1	0.00023	A	1

Table S2. Soft-SAFT molecular parameters of *n*-alkanes used in this work, as transferred from previous work.[9]

Substance	m	σ (Å)	ε/k_B (K)
Ethane	1.392	3.728	147.2
n-butane	2.134	3.871	237.7

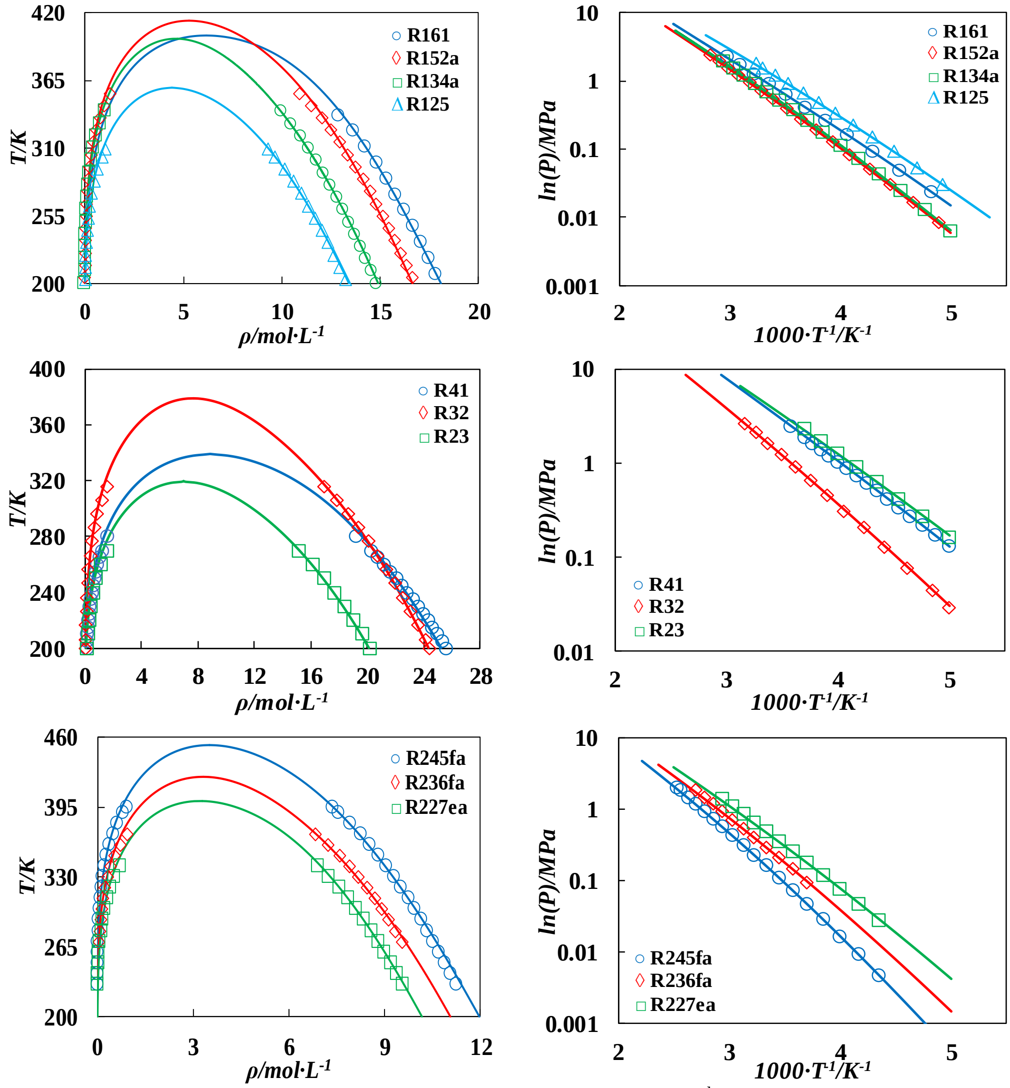

Fig. S1. Vapor pressure (right), and coexisting densities (left) for 3rd generation refrigerants studied in this work, with polar soft-SAFT EoS (solid lines), compared to experimental data[2,10] (symbols).

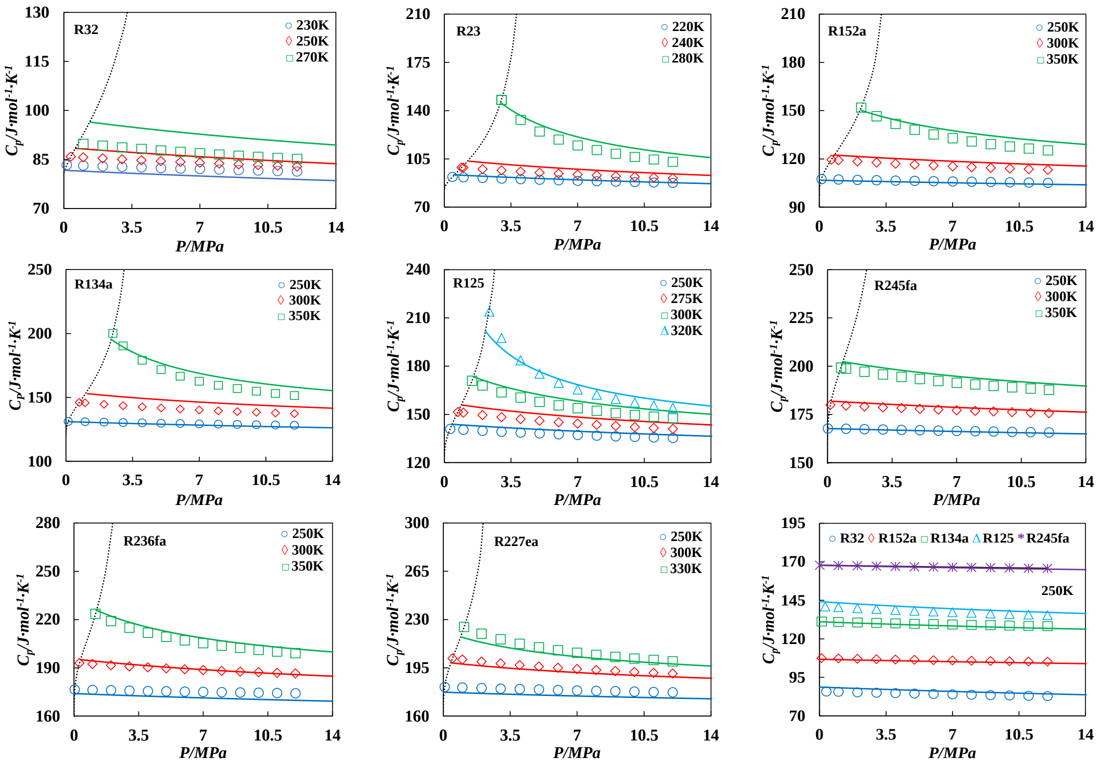

Fig. S2. Isobaric heat capacities of 3rd generation refrigerants predicted with polar soft-SAFT EoS (solid lines), compared to experimental data[2,11–13] (symbols).

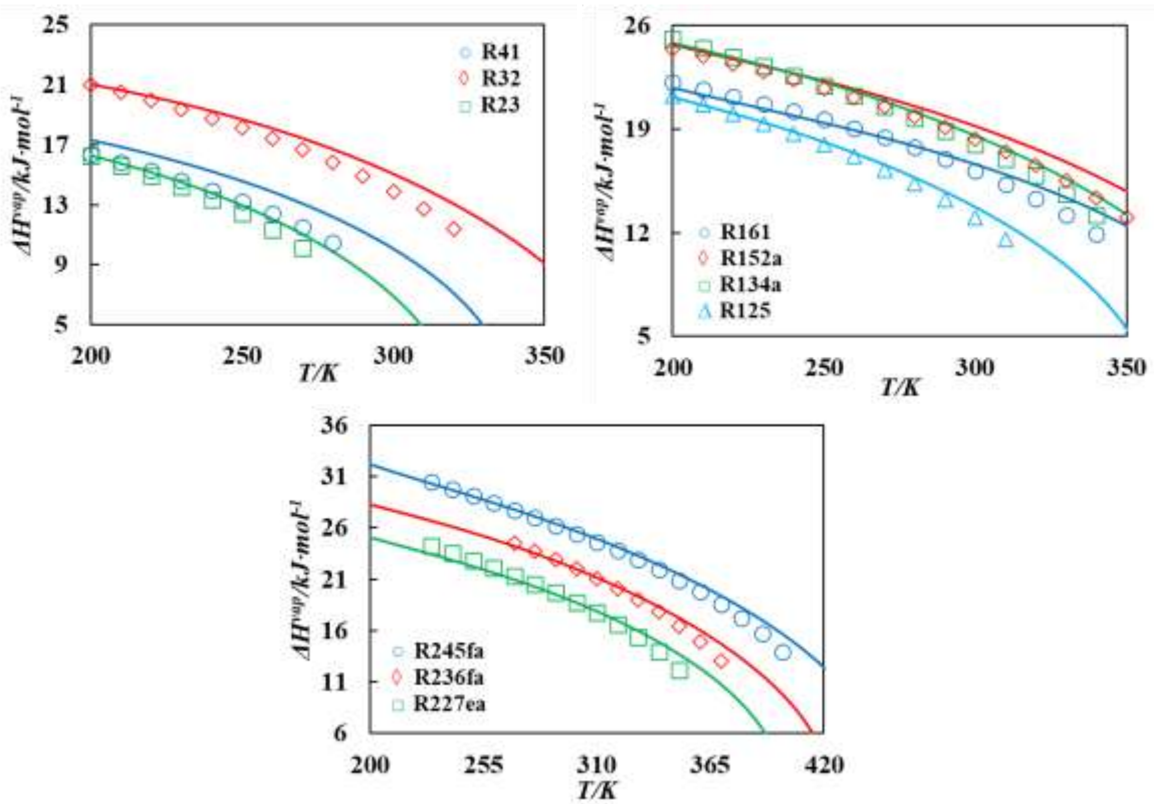

Fig. S3. Enthalpy of vaporization of 3rd generation refrigerants predicted with polar soft-SAFT EoS (solid lines), compared to experimental data[2] (symbols).

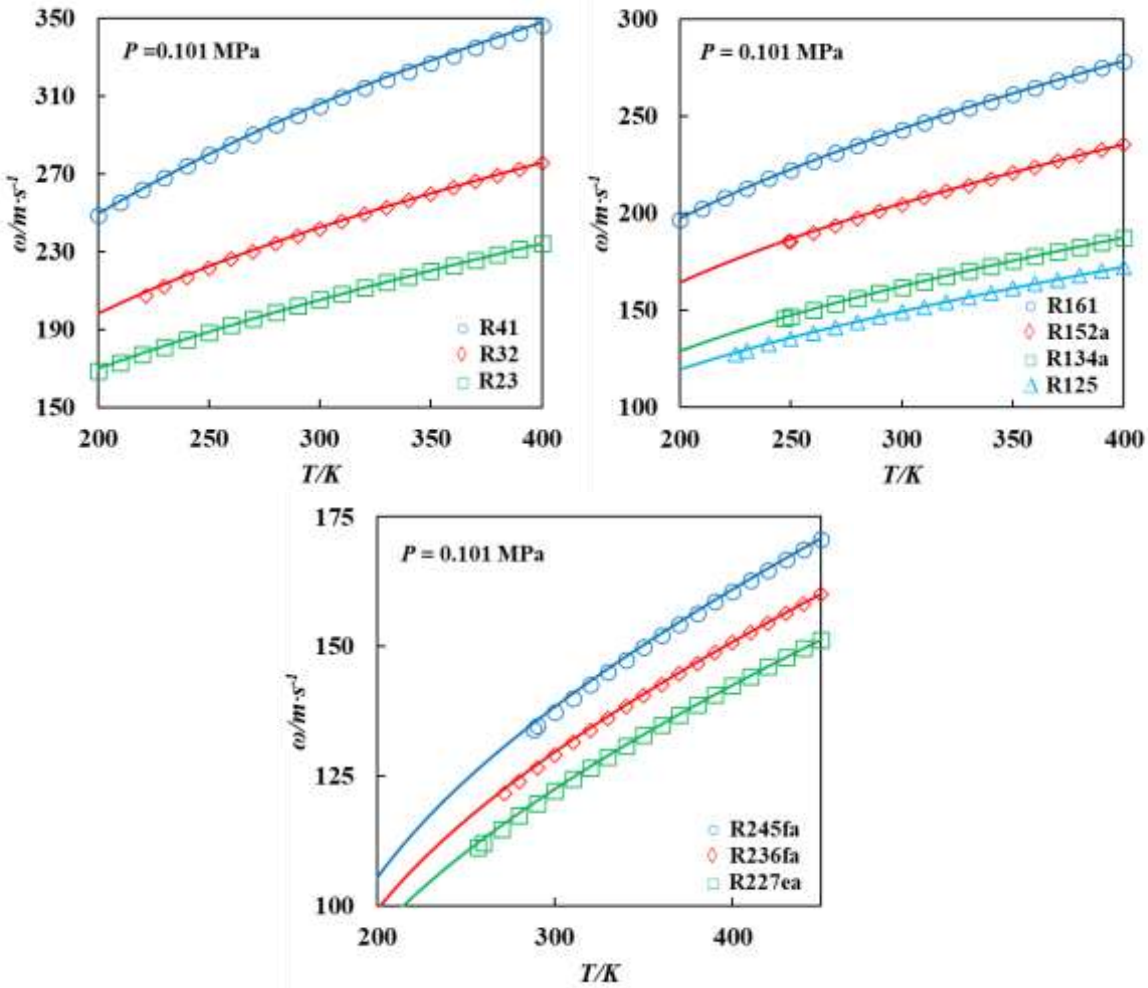

Fig. S4. Speed of sound of 3rd generation refrigerants predicted with polar soft-SAFT EoS (solid lines), compared to experimental data[2] (symbols).

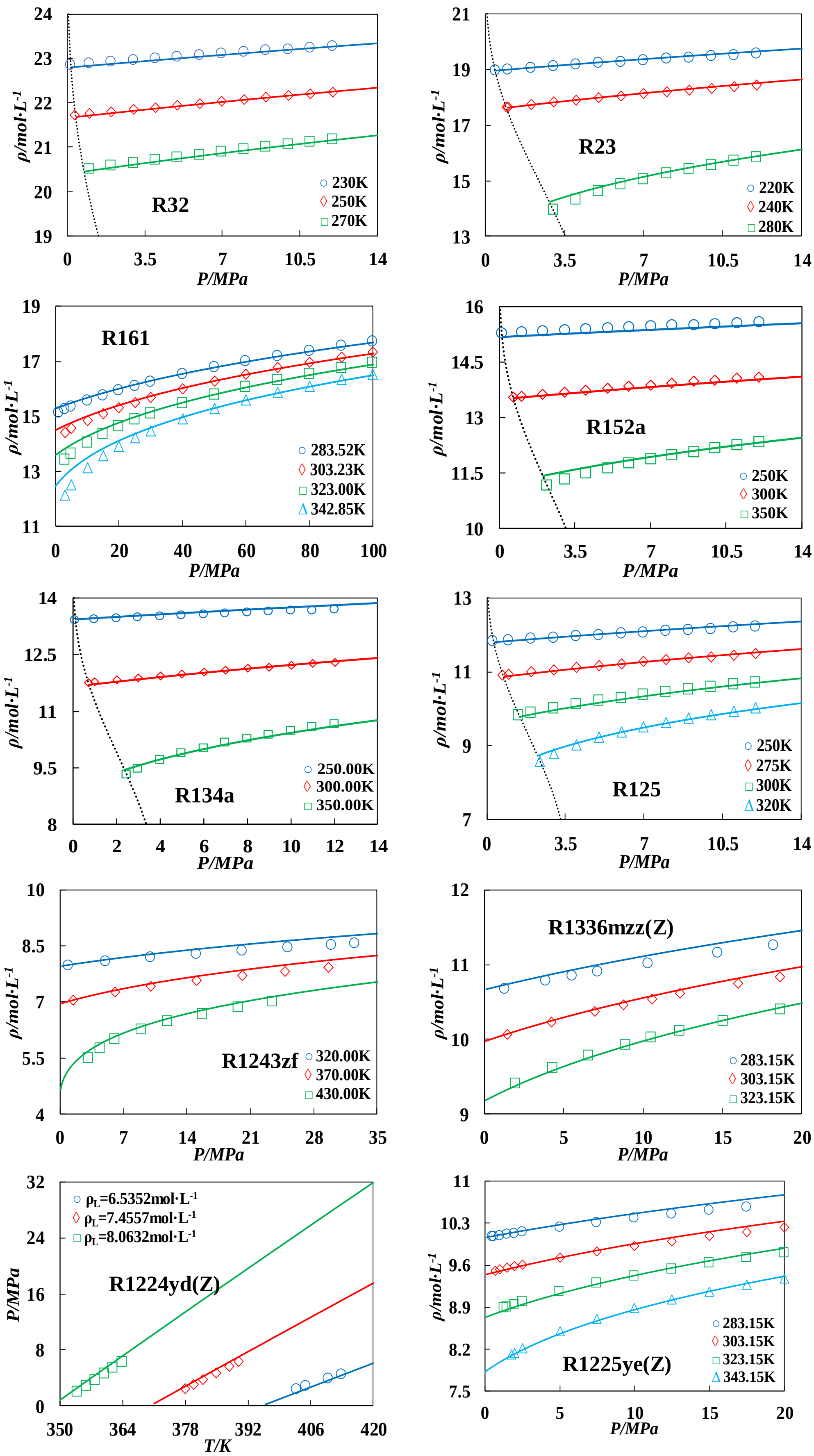

Fig. S5. Single-phase density of 3rd and 4th generation refrigerants predicted with polar soft-SAFT EoS (solid lines), compared to experimental data[2,14–18] (symbols).

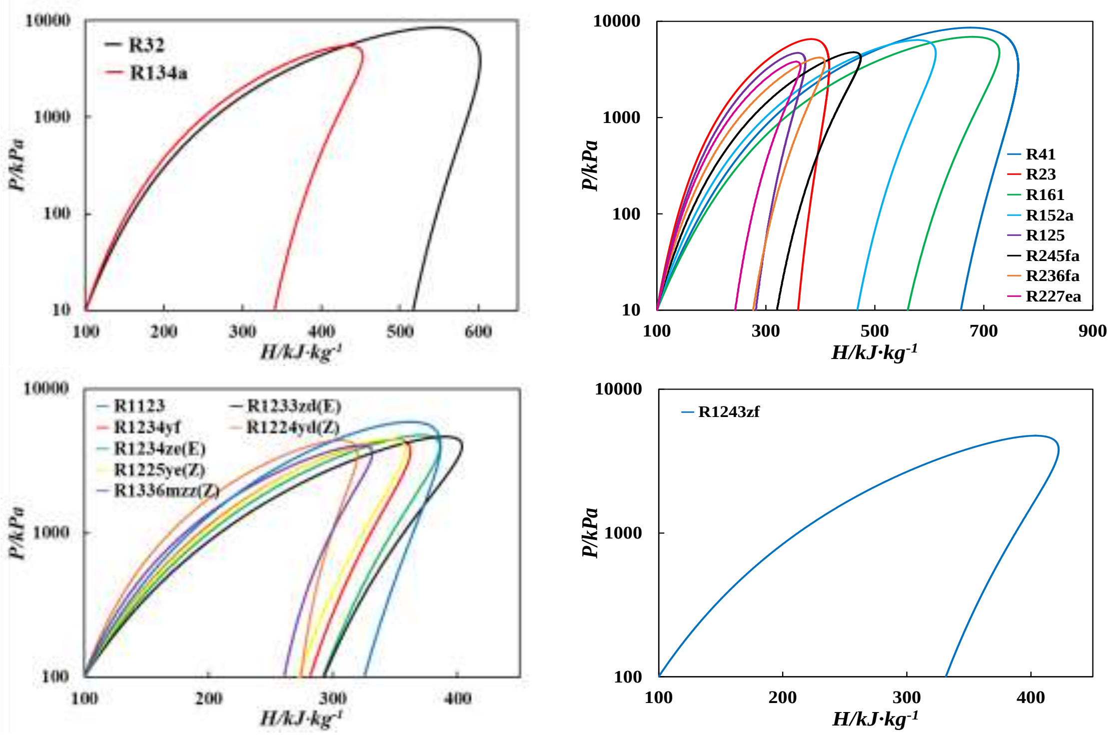

Fig. S6. Polar soft-SAFT predicted *PH* diagrams for the eighteen refrigerants modelled in this work.

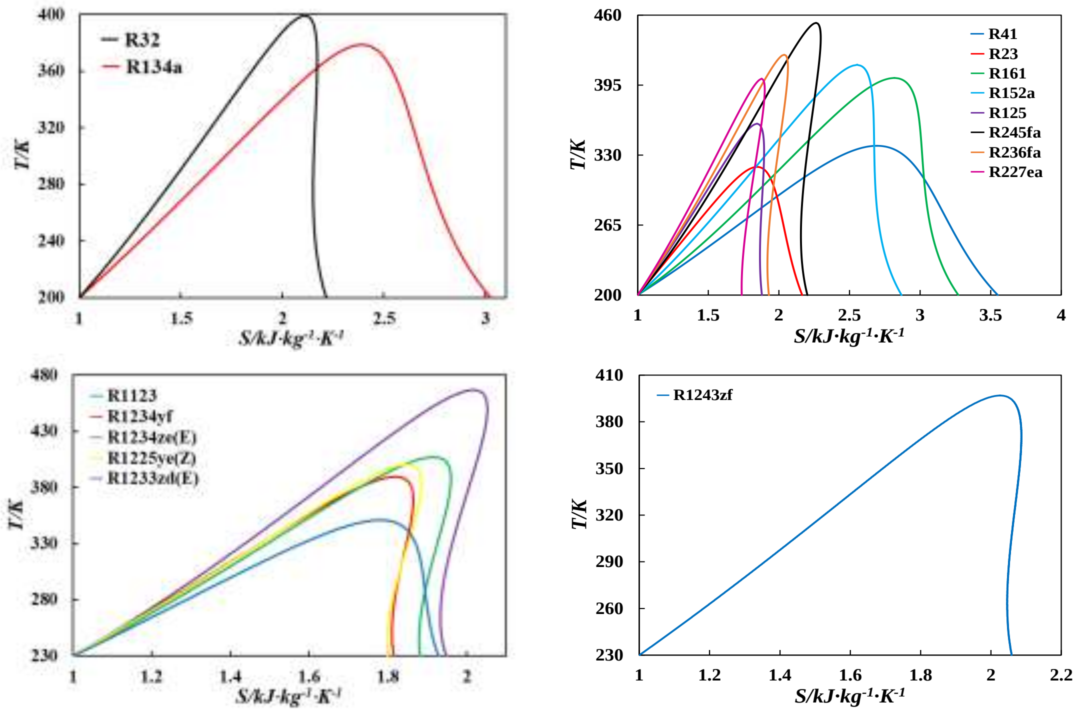

Fig. S7. Polar soft-SAFT predicted *TS* diagrams for sixteen refrigerants modeled in this work. Notice, predictions for R1336mzz(Z) and R1224yd(Z) cannot be obtained due to unavailability of ideal gas entropy for these refrigerants.

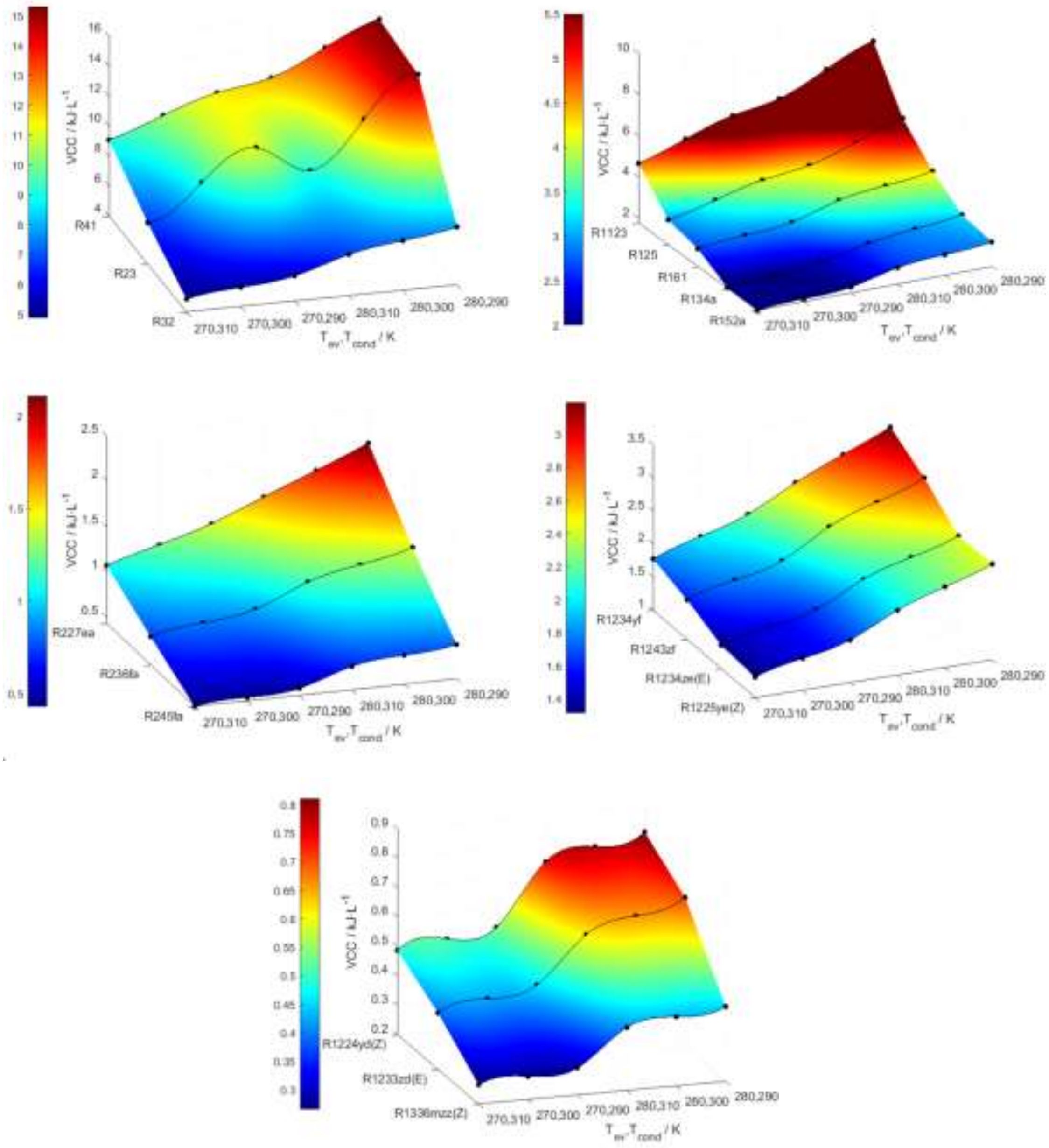

Fig. S81. VCC simulated at variable evaporator and condenser conditions for refrigerants modeled in this work

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