Taking 1-Chloropropane as an example, its topological index S is calculated as follows:

1. Numbering the atoms (except for hydrogen atoms) in molecular structure according to IUPAC systems.

C——C——C——Cl

3 2 1 4

2. Constructing the distance matrix D_w:

$$D_w = \begin{bmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 3 \\ 1 & 2 & 3 & 0 \end{bmatrix}$$

The interatomic bond distance is set as follows: singe bond, 1; double bond, 2; triple bond, 3; aromatic bond, 1.5, the a_{ij} in the matrix represents the overall distance between atom i and j.

3. Constructing the vertex weights matrix D_V:

$$D_V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 12 \end{bmatrix}$$

Vertex weights (V) are based on the atomic numbers of the vertices. The algorithm is V = 1 + (atomic no. of heteroatom – atomic no. of carbon). Thus, the vertex weights for the seven reactive elements of the second quantum level of the periodic chart are as follows: Li, -2; Be, -1; B, 0; C, 1; N, 2; O, 3; F, 4. The vertex weights matrix utilizes only its principal diagonal to record the V data.

4. Constructing the valency matrix Dv and valency vector v:

$$D_v = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

$$v = [2, 2, 1, 4]$$

The edge count about each hydrogen-suppressed vertex supplied a portion of the valence information. The algorithm is v = edge count about each hydrogen-suppressed vertex. For those heteratoms lying to the left of carbon in the periodic chart, each missing electron pair contributed -1 to the total valence of the heteroatom. Thus, all the heteroatoms in the second quantum level connected by a single bond to one carbon atom had the v numbers: Li, -2; Be, -1; B, 0; N, 2; 0, 3; F, 4.

So the topological index of 1-Chloropropane is calculated as follows:

$$D_{vVw} = D_v D_V D_w = \begin{bmatrix} 0 & 2 & 4 & 2 \\ 2 & 0 & 2 & 4 \\ 2 & 1 & 0 & 3 \\ 48 & 96 & 144 & 0 \end{bmatrix}$$

$$\mathrm{MTI}' = \sum_{i=1}^{N} (v D_{vVw})_i = \sum_{i=1}^{N} \left([2, 2, 1, 4] * \begin{bmatrix} 0 & 2 & 4 & 2 \\ 2 & 0 & 2 & 4 \\ 2 & 1 & 0 & 3 \\ 48 & 96 & 144 & 0 \end{bmatrix} \right) = 1190$$

$$\mathrm{GM} = 0$$

$$\mathrm{S} = \mathrm{MTI'} + \mathrm{GM} = 1190$$

5. Geometric modification number (GM)

The geometries about a pair of vertices responsible for geometric isomerism were indicated by geometric factors (GF) of +1 and +1 for Z (cis) geometry, and -1, -1 for E (trans) geometry. All other vertices in the graph were assigned GF values of zero. Those factors were used to quantify

the geometric isomerism of a given compound. Taking 1,2-Difluoroethene as an example:

F——C===C——F
3 1 2 4

$$D_w = \begin{bmatrix} 0 & 2 & 1 & 3 \\ 2 & 0 & 3 & 1 \\ 1 & 3 & 0 & 4 \\ 3 & 1 & 4 & 0 \end{bmatrix}, D_V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}, D_v = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

$$D_{vVw} = D_v D_V D_w = \begin{bmatrix} 0 & 6 & 3 & 9 \\ 6 & 0 & 9 & 3 \\ 16 & 48 & 0 & 64 \\ 48 & 16 & 64 & 0 \end{bmatrix}$$

$$\mathrm{MTI}' = \sum_{i=1}^{N} (vD_{vVw})_i = \sum_{i=1}^{N} \left([3,3,4,4] * \begin{bmatrix} 0 & 6 & 3 & 9 \\ 6 & 0 & 9 & 3 \\ 16 & 48 & 0 & 64 \\ 48 & 16 & 64 & 0 \end{bmatrix} \right) = 1132$$

$$M_{GF,Z} = \begin{bmatrix} +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, M_{GF,E} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathrm{GM_Z} = \sum_{i=1}^{N} M_{GF,Z}(D_{vVw} + D_{vVw}^T) = 176$$

$$\mathrm{GM_E} = \sum_{i=1}^{N} M_{GF,E}(D_{vVw} + D_{vVw}^T) = -176$$

The GM number for (Z)-1,2-Difluoroethene is added to the MTI' value of 1132, the sum is the S index for (Z)-1,2-Difluoroethene, 1308. The S index for (E)-1,2-Difluoroethene is attained in the same manner: S = 1132-176 = 956.

Table S1 shows the topological indices of all 155 working fluids in this research.

Table S1 Topological indices of working fluids

Name	S	Formula
Methane	0	CH4
Fluoromethane	65	CH3F
Difluoromethane	392	CH2F2
Trifluoromethane	987	CHF3
Tetrafluoromethane	1856	CF4
Iodomethane	769	CH3I
Bromomethane	481	CH3Br
Dibromomethane	2888	CH2Br2

Chloromethane	193	CH3Cl
Dichloromethane	1160	CH2Cl2
Trichloromethane	2907	CHCl3
Tetrachloromethane	5440	CCl4
Bromodifluoromethane	3067	CHBrF2
Bromochlorodifluoromethane	5664	CBrClF2
Bromotrifluoromethane	4768	CBrF3
Iodotrifluoromethane	6784	CF3I
Chlorofluoromethane	776	CH2ClF
Chlorodifluoromethane	1627	CHClF2
Chlorotrifluoromethane	2752	CClF3
Dichlorofluoromethane	2267	CHCl2F
Dichlorodifluoromethane	3648	CCl2F2
Trichlorofluoromethane	4544	CCl3F
Ethane	2	C2H6
Chloroethane	587	C2H5Cl
Fluoroethane	203	C2H5F
1,1-Difluoroethane	672	C2H4F2
1,1,1-Trifluoroethane	1415	C2H3F3
1,1,2-Trifluoroethane	1669	C2H3F3
1,1,1,2-Tetrafluoroethane	2816	C2H2F4
1,1,2,2-Tetrafluoroethane	2942	C2H2F4
Pentafluoroethane	4497	C2HF5
Hexafluoroethane	6464	C2F6
Bromoethane	1451	C2H5Br
1-Chloro-1,1-difluoroethane	2311	C2H3ClF2
Chloropentafluoroethane	8512	C2ClF5
1,1-Dichloro-1-fluoroethane	3207	C2H3Cl2F
1,1-Dichloro-1,2,2,2-tetrafluoroethane	10560	C2Cl2F4
2,2-Dichloro-1,1,1-trifluoroethane	8080	C2HCl2F3
1,2-Dichloro-1,1,2,2-tetrafluoroethane	10560	C2Cl2F4
1,1,1-Trichloroethane	4103	C2H3Cl3
1,1,2,2-Tetrachloro-1,2-difluoroethane	14656	C2Cl4F2
1,1,1,2-Tetrachloro-2,2-difluoroethane	14656	C2Cl4F2
1,1,2-Trichlorotrifluoroethane	12608	C2Cl3F3
2-Chloro-1,1,1,2-tetrafluoroethane	6289	C2HClF4
1,2-Dibromotetrafluoroethane	19776	C2Br2F4
Propane	14	C3H8
1-Bromopropane	2918	C3H7Br
1-Chloropropane	1190	C3H7Cl
2-Chloropropane	997	C3H7Cl
2-Fluoropropane	357	C3H7F
1,1,1,3,3-Pentafluoropropane	6382	C3H3F5
1,1,2,2,3-Pentafluoropropane	5956	C3H3F5

1,1,1,2,2,3-Hexafluoropropane	8276	C3H2F6
1,1,1,2,3,3-Hexafluoropropane	8741	C3H2F6
1,1,1,3,3,3-Hexafluoropropane	8984	C3H2F6
1,1,1,2,3,3,3-Heptafluoropropane	11751	C3HF7
Perflutren	14816	C3F8
1,2-Dichloro-1,1,2-trifluoropropane	9552	C3H3Cl2F3
Butane	44	C4H10
Isobutane	42	C4H10
1,1,1,2,2,3,3,4-Octafluorobutane	17636	C4H2F8
1,1,1,2,2,4,4,4-Octafluorobutane	19052	C4H2F8
1,1,1,2,2,3,3,4,4-Nonafluorobutane	22542	C4HF9
Perflubutane	27776	C4F10
1-Methoxybutane	278	C5H12O
Vinyl butyl ether	627	C6H12O
2,2-Dimethylbutane	170	C6H14
2,3-Dimethylbutane	170	C6H14
2,2,3-Trimethylbutane	276	C7H16
Pentane	100	C5H12
Isopentane	94	C5H12
Neopentane	92	C5H12
2-Methylpentane	182	C6H14
3-Methylpentane	172	C6H14
2,2-Dimethylpentane	296	C7H16
2,4-Dimethylpentane	302	C7H16
3,3-Dimethylpentane	274	C7H16
3-Ethylpentane	276	C7H16
2,2,3-Trimethylpentane	424	C8H18
2,2,4-Trimethylpentane	460	C8H18
2,3,3-Trimethylpentane	412	C8H18
2,3,4-Trimethylpentane	426	C8H18
3-Ethyl-2-methylpentane	416	C8H18
3-Ethyl-3-methylpentane	404	C8H18
Hexane	190	C6H14
Perflexane	71488	C6F14
2-Methylhexane	314	C7H16
3-Methylhexane	298	C7H16
2,2-Dimethylhexane	478	C8H18
2,5-Dimethylhexane	488	C8H18
3,3-Dimethylhexane	434	C8H18
Heptane	322	C7H16
Perfluoroheptane	104984	C7F16
2-Methylheptane	498	C8H18
3-Methylheptane	468	C8H18
4-Methylheptane	458	C8H18

Octane	504	C8H18
Perfluorooctane	142976	C8F18
Ethylene	16	C2H4
Fluoroethylene	303	C2H3F
1,1-Difluoroethylene	864	C2H2F2
2-Chloro-1,1-difluoroethylene	3777	C2HClF2
1-Chloro-1,2,2-trifluoroethene	5696	C2ClF3
1,1-Dichloroethene	2400	C2H2Cl2
Tetrafluoroethylene	3904	C2F4
(Z)-1,2-Dichloroethene	3846	C2H2Cl2
(E)-1,2-Dichloroethene	2838	C2H2Cl2
Ethoxyethylene	255	C4H8O
Propylene	51	C3H6
3-Chloro-1-propene	1445	C3H5Cl
3,3,3-Trifluoropropene	2373	C3H3F3
(E)-1,2,3,3-Tetrafluoropropene	4604	C3H2F4
2,3,3,3-Tetrafluoropropene	4032	C3H2F4
(Z)-1,3,3,3-Tetrafluoropropene	5460	C3H2F4
(E)-1,3,3,3-Tetrafluoropropene	4520	C3H2F4
1,1,3,3,3-Pentafluoropropene	7911	C3HF5
(Z)-1,2,3,3,3-Pentafluoropropene	7758	C3HF5
(E)-1,2,3,3,3-Pentafluoropropene	6636	C3HF5
Isobutylene	108	C4H8
1,2-Propadiene	112	C3H4
1-Butene	108	C4H8
(Z)-2-Butene	180	C4H8
(E)-2-Butene	68	C4H8
2-Methyl-1-butene	191	C5H10
2-Methyl-2-butene	225	C5H10
3-Methyl-1-butene	187	C5H10
Hexafluoro-1,3-butadiene	15680	C4F6
1,3-Butadiene	188	C4H6
1-Pentene	199	C5H10
(Z)-2-Pentene	305	C5H10
(E)-2-Pentene	141	C5H10
4-Methyl-1-pentene	318	C6H12
1-Hexene	332	C6H12
1,5-Hexadiene	490	C6H10
1-Heptene	515	C7H14
1-Octene	1036	C8H16
Dimethyl ether	30	C2H6O
1,1,3,3-Tetrafluorodimethyl ether	4414	C2H2F4O
Pentafluorodimethyl ether	6576	C2HF5O
trifluoro(methoxy)methane	2124	C2H3F3O

Pentafluoroethyl methyl ether	6766	C3H3F5O
2-(Difluoromethoxy)-1,1,1-trifluoroethane	8784	C3H3F5O
1,1,1-Trifluoro-2-(trifluoromethoxy)ethane	14128	C3H2F6O
Dimethoxymethane	212	C3H8O2
Heptafluoroisopropyl methyl ether	15420	C4H3F7O
Heptafluoro-1-methoxypropane	14190	C4H3F7O
1,1,1,2,2-Pentafluoro-3-(trifluoromethoxy)propane	24124	C4H2F8O
Ethoxyethane	148	C4H10O
1,2-Dimethoxyethane	366	C4H10O2
Methyl tert-butyl ether	234	C5H12O
2,2-Dimethoxypropane	450	C5H12O2
Ethyl propyl ether	278	C5H12O
Tert-Butyl ethyl ether	376	C6H14O
Dipropyl ether	418	C6H14O