

Thermal conductivity of liquids: Aromatic compounds containing oxygen

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THE PREPARATION OF THIS DATA ITEM

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THERMAL CONDUCTIVITY OF LIQUIDS: AROMATIC COMPOUNDS CONTAINING OXYGEN

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Data sheets for each of the liquids are given in the following order:

Formula	Name	Alternative Name(s)	
AROMATIC ALCOHOLS			
1. C_6H_5OH	Phenol	Hydroxybenzene Carbolic acid	7
2. $2-CH_3C_6H_4OH$	2-Methylphenol	2-Hydroxytoluene o-Cresol	8
3. $3-CH_3C_6H_4OH$	3-Methylphenol	3-Hydroxytoluene m-Cresol	9
4. $4-CH_3C_6H_4OH$	4-Methylphenol	4-Hydroxytoluene p-Cresol	10
5. $2,3-(CH_3)_2C_6H_3OH$	2,3-Dimethylphenol	2,3-Xylenol	11
6. $2,4-(CH_3)_2C_6H_3OH$	2,4-Dimethylphenol	2,4-Xylenol	12
7. $2,5-(CH_3)_2C_6H_3OH$	2,5-Dimethylphenol	2,5-Xylenol	13
8. $2,6-(CH_3)_2C_6H_3OH$	2,6-Dimethylphenol	2,6-Xylenol	14
9. $3,4-(CH_3)_2C_6H_3OH$	3,4-Dimethylphenol	3,4-Xylenol	15
10. $3,5-(CH_3)_2C_6H_3OH$	3,5-Dimethylphenol	3,5-Xylenol	16

Formula	Name	Alternative Name(s)
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PHENYL ALKANOLS and HALOGENATED AROMATIC ALCOHOLS

11. $C_6H_5CH_2OH$	Benzyl alcohol	α -Hydroxytoluene 7-Hydroxytoluene (Hydroxymethyl)benzene Phenylmethanol Phenyl carbinol	17
12. $2-ClC_6H_4OH$	2-Chlorophenol	<i>o</i> -Chlorophenol	18
13. $3-ClC_6H_4OH$	3-Chlorophenol	<i>m</i> -Chlorophenol	19
14. $4-ClC_6H_4OH$	4-Chlorophenol	<i>p</i> -Chlorophenol	20

AROMATIC ETHERS

15. $CH_3OC_6H_5$	Methyl phenyl ether	Methoxybenzene Anisole	21
16. $CH_3CH_2OC_6H_5$	Ethyl phenyl ether	Ethoxybenzene Phenetole	22
17. $C_6H_5OC_6H_5$	Diphenyl ether	Phenoxybenzene Phenyl ether	23

AROMATIC ESTERS

18. $C_6H_5COOCH_3$	Methyl benzoate	Methyl benzenecarboxylate	24
19. $C_6H_5COOCH_2CH_3$	Ethyl benzoate	Ethyl benzenecarboxylate	25
20. $2-C_6H_4(COOCH_3)_2$	Dimethyl phthalate	Dimethyl benzene-1,2-dicarboxylate	26
21. $2-C_6H_4(COOCH_2CH_3)_2$	Diethyl phthalate	Diethyl benzene-1,2-dicarboxylate	28
22. $2-C_6H_4(COO[CH_2]_2CH_3)_2$	Dipropyl phthalate	Dipropyl benzene-1,2-dicarboxylate	29
23. $2-C_6H_4(COOCH(CH_3)_2)_2$	Diisopropyl phthalate	Bis(1-methylethyl) benzene-1,2-dicarboxylate	30
24. $2-C_6H_4(COO[CH_2]_3CH_3)_2$	Dibutyl phthalate	Dibutyl benzene-1,2-dicarboxylate	31
25. $2-C_6H_4(COOCH_2CH(CH_3)_2)_2$	Diisobutyl phthalate	Bis(2-methylpropyl) benzene-1,2-dicarboxylate	33
26. $2-C_6H_4(COO[CH_2]_5CH_3)_2$	Diethyl phthalate	Diethyl benzene-1,2-dicarboxylate	34
27. $2-C_6H_4(COO[CH_2]_6CH_3)_2$	Diheptyl phthalate	Diheptyl benzene-1,2-dicarboxylate	35
28. $2-C_6H_4(COOCH_2CH(CH_2CH_3)[CH_2]_3CH_3)_2$	Bis(2-ethylhexyl) phthalate	Bis(2-ethylhexyl) benzene-1,2-dicarboxylate	36
29. $2-C_6H_4(COO[CH_2]_9CH_3)_2$	Didecyl phthalate	Didecyl benzene-1,2-dicarboxylate	37

AROMATIC ALDEHYDES and KETONES

30. C_6H_5CHO	Benzaldehyde	Benzenecarbaldehyde	38
31. $CH_3COC_6H_5$	Methyl phenyl ketone	Acetophenone	39

THERMAL CONDUCTIVITY OF LIQUIDS: AROMATIC COMPOUNDS CONTAINING OXYGEN

1. INTRODUCTION

This Item presents values of thermal conductivity at saturation pressure, in tabular form, for liquid aromatic compounds containing oxygen.

The data on which these recommended values of thermal conductivity are based are the most reliable available and the temperature range covered is from the melting temperature to approximately 0.9 of the critical temperature. Quantities are expressed in SI units and conversion factors to other units are provided in Section 3.

Section 4 describes the procedure used to obtain the values of thermal conductivity presented and indicates the effect of pressure. Section 5 gives an explanation of the Tables and indicates the uncertainties in the values presented in them.

References to sources of supplementary information are given in Section 6. The data sources for each particular compound are listed on the appropriate data sheet.

2. NOTATION AND UNITS

The SI unit of thermal conductivity is the watt per metre kelvin (W/m K). A convenient submultiple SI unit for the range of thermal conductivity in this Item is the milliwatt per metre kelvin (mW/m K); hence that is the unit adopted here.

A	constant for each liquid in Equation (4.2)	mW/m K
A'	constant for each liquid in Equation (4.1)	mW/m K
B, C, D	non-dimensional constants for each liquid in Equation (4.2)	–
p	pressure	N/m ² (Pa)
T	kelvin temperature	K
t	Celsius temperature, $T - 273.15$	°C
λ	thermal conductivity	mW/m K

Subscripts

c	denotes value at the critical point
p	denotes value at pressure p
r	denotes reduced quantity, <i>e.g.</i> $T_r = T/T_c$.

3. CONVERSION FACTORS

$$\begin{aligned}
 1 \text{ mW/m K} &= 0.8598 \times 10^{-3} \text{ kcal/m h } ^\circ\text{C}^* \\
 &= 2.3885 \times 10^{-6} \text{ cal/cm s } ^\circ\text{C}^* \\
 &= 0.5778 \times 10^{-3} \text{ Chu/ft h } ^\circ\text{C}^* \\
 &= 0.5778 \times 10^{-3} \text{ Btu/ft h } ^\circ\text{F}^* \\
 &= 6.9335 \times 10^{-3} \text{ Btu in/ft}^2 \text{ h } ^\circ\text{F}^*
 \end{aligned}$$

$$\begin{aligned}
 10^5 \text{ N/m}^2 &= 1 \text{ bar} \\
 &= 14.5038 \text{ lbf/in}^2 \\
 &= 1.0197 \text{ kgf/cm}^2 \\
 &= 0.9869 \text{ atm} \\
 &= 750.062 \text{ mmHg.}
 \end{aligned}$$

* The values used for the calorie and British Thermal Unit are International Table values.

4. THERMAL CONDUCTIVITY

4.1 Thermal Conductivity at Saturation Pressure

In Reference 2 Riedel showed that the experimental data for the thermal conductivity of normal (that is unassociated) liquids along the saturation line could be represented by the equation:

$$\lambda = A' [1 + (20/3)(1 - T_r)^{2/3}]. \quad (4.1)$$

The range of applicability of Equation (4.1) is limited for most compounds. For the liquids considered in this Item a good representation of the data* between the melting temperature and $T_r = 0.9$ is obtained from the equation:

$$\lambda = A [1 + B(1 - T_r)^{1/3} + C(1 - T_r)^{2/3} + D(1 - T_r)]. \quad (4.2)$$

Measurements of thermal conductivity have been made for relatively few liquids at $T_r > 0.9$ and so, because of the uncertain variation of thermal conductivity in the critical region, data are presented only for temperatures up to $T_r = 0.9$. The equation extrapolates in a physically realistic manner to within a few kelvin of the critical point.

The critical temperatures for these compounds have either been taken from ESDU 81025, 81042, 94001, 95016 (References 7, 8, 11 and 12) or estimated from correlations of ESDU values with chemical structure. In this Item, the critical temperatures should be regarded as correlating parameters only and should not be taken as a source of accurate values.

The derived values of A , B , C and D given in Table 7.1 are a correlated set of values giving the best fit to the experimental data, not only as individual compounds but also as members of their chemical series. This method of correlating data for a series of compounds has been described in References 5 and 6. For all the phenols† in this Item, it was found that B , C and D remain constant, as was observed for other hydrogen bonded compounds such as the aliphatic alcohols and amines. For the ethers, esters, aldehydes

* Experimental data at temperatures below the normal boiling temperature, t_b , are often at 1 atm pressure. As indicated in Section 4.2 the difference between values of λ at 1 atm pressure and at saturation pressure below t_b is not significant.

† $B = 3.0$, $C = -6.5$, $D = 4.7$ for phenols.

and ketones in this Item, it was found that C and D are directly related to B^* , as was observed for other non-hydrogen-bonded compounds such as the alkanes. Correlated values of the constants A , B , C and D were used to estimate constants for liquids for which no experimental data exist. Using these values with the values of T_c given in Table 7.1, values of λ in mW/m K have been calculated for each compound from Equation (4.2) and are presented in the data sheets.

4.2 Effect of Pressure

At temperatures up to the normal boiling point, the effect of pressure from the saturation pressure to 50×10^5 N/m² (up to 50 atm) is to increase the thermal conductivity by approximately 1 per cent and, for most practical purposes, values at saturation pressure may be taken as equal to those at atmospheric pressure.

Reference 1 gives measurements of thermal conductivity for a number of liquids up to $12\,000 \times 10^5$ N/m² ($\approx 12\,000$ atm) at 30 °C and 75 °C. A generalised correlation of these results is given in Reference 3, but a knowledge of the critical pressure of the substance is required for its use.

For pressures up to 500×10^5 N/m² (≈ 500 atm) between the melting temperature and the normal boiling point a very approximate relationship:

$$\lambda_p/\lambda \approx 1 + 0.2p \times 10^{-8}, \quad (4.3)$$

may be used where λ_p is the thermal conductivity at pressure p and λ is the thermal conductivity at a pressure of 10^5 N/m² (≈ 1 atm), both at the same temperature.

5. EXPLANATION OF TABLES

The constants of Equation (4.2) are given in Table 7.1 and on the data sheets. Values of the thermal conductivity are given in the data sheets at 10 kelvin intervals in K and °C, from within 10 kelvin of the melting temperature, or an appropriate starting temperature where the melting temperature is unknown, to a temperature corresponding with $T_r \approx 0.9$.

The sources are given in the data sheets and extrapolated values are indicated in parentheses.

For uniformity and ease of interpolation the data are presented and can be read to more significant digits than is warranted by their estimated accuracy.

The experimental data from the most reliable individual sources have a repeatability of about ± 1 per cent although differences in technique used by different workers (and possibly also in the purity of samples) can increase the uncertainty in the absolute values to about ± 2 per cent. However, such reliable data are not available for all the compounds considered, nor over the whole temperature range covered. Although it is considered that the correlation procedures adopted keep the errors in the values presented to a minimum, the user should in general allow for an uncertainty of ± 5 per cent[†] unless the value in the data sheet is truncated to a whole number. Where whole numbers are given the uncertainty increases to ± 10 per cent.

Some fluids have poor thermal stability coupled with a high critical temperature. Values have been tabulated for all fluids up to $T_r \approx 0.9$ but many of these fluids will decompose at elevated temperatures. As most compounds will decompose rapidly at temperatures above about 300 °C, uncertainties of greater than ± 10 per cent may occur for temperatures ≥ 573 K.

* $C = 1 - 3B$ and $D = 3B$ for ethers, esters, aldehydes and ketones.

† Dimethyl and dibutyl phthalate have been considered suitable for calibrating or checking experimental equipment. Values reported are believed to be accurate to within ± 2 per cent over the range 20 to 200 °C.

6. REFERENCES

The references given are recommended sources of information supplementary to that in this Item.

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7. TABLES

TABLE 7.1 Constants for Equation (4.2)

Compound	T_c	A	B	C	D	Range of Applicability		
	K	mW/m K				°C		
1. Phenol	694.25	93.0	3.0	-6.5	4.7	40	to	360
2. 2-Methylphenol	697.55	88.6	3.0	-6.5	4.7	30	to	360
3. 3-Methylphenol	705.75	88.0	3.0	-6.5	4.7	10	to	370
4. 4-Methylphenol	704.55	86.0	3.0	-6.5	4.7	30	to	370
5. 2,3-Dimethylphenol	722.8	85.2	3.0	-6.5	4.7	70	to	390
6. 2,4-Dimethylphenol	707.6	84.5	3.0	-6.5	4.7	20	to	370
7. 2,5-Dimethylphenol	706.9	84.5	3.0	-6.5	4.7	70	to	370
8. 2,6-Dimethylphenol	701.	85.2	3.0	-6.5	4.7	40	to	370
9. 3,4-Dimethylphenol	729.8	83.2	3.0	-6.5	4.7	60	to	390
10. 3,5-Dimethylphenol	715.6	83.2	3.0	-6.5	4.7	60	to	380
11. Benzyl alcohol	674.15	96.0	3.0	-6.5	4.7	-20	to	340
12. 2-Chlorophenol	675.	82.5	3.0	-6.5	4.7	10	to	340
13. 3-Chlorophenol	720.	81.4	3.0	-6.5	4.7	30	to	380
14. 4-Chlorophenol	730.	79.3	3.0	-6.5	4.7	40	to	390
15. Methyl phenyl ether	645.6	64.0	1.4	-3.2	4.2	-40	to	320
16. Ethyl phenyl ether	652.5	64.0	1.2	-2.6	3.6	-30	to	320
17. Diphenyl ether	766.8	57.0	1.5	-3.5	4.5	20	to	430
18. Methyl benzoate	687.15	61.3	1.4	-3.2	4.2	-10	to	350
19. Ethyl benzoate	692.15	60.4	1.3	-2.9	3.9	-40	to	360
20. Dimethyl phthalate	760.15	67.0	1.0	-2.0	3.0	0	to	420
21. Diethyl phthalate	762.15	65.0	0.9	-1.7	2.7	-10	to	420
22. Dipropyl phthalate	775.15	66.0	0.7	-1.1	2.1	-30	to	430
23. Diisopropyl phthalate	760.15	62.0	0.7	-1.1	2.1	-30	to	420
24. Dibutyl phthalate	786.15	66.0	0.6	-0.8	1.8	-30	to	440
25. Diisobutyl phthalate	765.15	62.0	0.6	-0.8	1.8	-50	to	420
26. Dihexyl phthalate	802.	67.0	0.5	-0.5	1.5	-40	to	460
27. Diheptyl phthalate	808.	67.5	0.5	-0.5	1.5	-40	to	460
28. Bis(2-ethylhexyl) phthalate	802.15	68.0	0.5	-0.5	1.5	-50	to	460
29. Didecyl phthalate	843.	68.2	0.5	-0.5	1.5	-50	to	490
30. Benzaldehyde	695.	70.0	1.0	-2.0	3.0	-60	to	360
31. Methyl phenyl ketone	704.15	67.0	1.0	-2.0	3.0	20	to	370

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C₆H₅OH PHENOL (HYDROXYBENZENE, CARBOLIC ACID)

$$\lambda = A[1 + B(1 - T_r)^{1/3} + C(1 - T_r)^{2/3} + D(1 - T_r)]$$

where

λ = thermal conductivity at saturation pressure (mW/m K)

$T_r = T/T_c$, T = temperature (K)

$T_c = 694.25$ K

$A = 93.0$, $B = 3.0$, $C = -6.5$, $D = 4.7$

T K	λ mW/m K	T K	λ mW/m K	t °C	λ mW/m K	t °C	λ mW/m K
310	156.	480	(140.4)	40	156.	210	(140.2)
320	155.3	490	(139.8)	50	154.9	220	(139.6)
330	154.1	500	(139.2)	60	153.8	230	(139.0)
340	153.0	510	(138.7)	70	152.6	240	(138.5)
350	151.9	520	(138.2)	80	151.5	250	(138.0)
360	150.8	530	(138.)	90	150.4	260	(138.)
370	149.7	540	(137.)	100	149.4	270	(137.)
380	148.7	550	(137.)	110	148.4	280	(137.)
390	147.7	560	(137.)	120	147.4	290	(137.)
400	146.7	570	(136.)	130	146.5	300	(136.)
410	145.8	580	(136.)	140	145.5	310	(136.)
420	144.9	590	(136.)	150	144.7	320	(136.)
430	144.1	600	(136.)	160	143.8	330	(136.)
440	143.3	610	(136.)	170	143.0	340	(136.)
450	142.5	620	(136.)	180	142.2	350	(136.)
460	141.7	630	(136.)	190	141.5	360	(136.)
470	141.0			200	140.8		

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2-CH₃C₆H₄OH 2-METHYLPHENOL (2-HYDROXYTOLUENE, o-CRESOL)

$$\lambda = A[1 + B(1 - T_r)^{1/3} + C(1 - T_r)^{2/3} + D(1 - T_r)]$$

where

λ = thermal conductivity at saturation pressure (mW/m K)

$T_r = T/T_c$, T = temperature (K)

$T_c = 697.55$ K

$A = 88.6$, $B = 3.0$, $C = -6.5$, $D = 4.7$

T K	λ mW/m K	T K	λ mW/m K	t °C	λ mW/m K	t °C	λ mW/m K
300	(150.)	470	(134.5)	30	150.	200	(134.3)
310	149.3	480	(133.9)	40	148.9	210	(133.7)
320	148.1	490	(133.3)	50	147.8	220	(133.1)
330	147.0	500	(132.7)	60	146.7	230	(132.6)
340	145.9	510	(132.2)	70	145.6	240	(132.1)
350	144.9	520	(131.7)	80	144.5	250	(131.6)
360	143.8	530	(131.)	90	143.5	260	(131.)
370	142.8	540	(131.)	100	142.5	270	(131.)
380	141.8	550	(131.)	110	141.5	280	(131.)
390	140.9	560	(130.)	120	140.6	290	(130.)
400	140.0	570	(130.)	130	139.7	300	(130.)
410	139.1	580	(130.)	140	138.8	310	(130.)
420	138.2	590	(130.)	150	138.0	320	(130.)
430	137.4	600	(130.)	160	137.2	330	(130.)
440	136.6	610	(130.)	170	136.4	340	(130.)
450	(135.9)	620	(130.)	180	(135.7)	350	(130.)
460	(135.2)	630	(130.)	190	(135.0)	360	(130.)

FILIPPOV, L.P.

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JAMIESON, D.T.

Unpublished data, National Engineering Laboratory, East Kilbride, UK.

3-CH₃C₆H₄OH 3-METHYLPHENOL (3-HYDROXYTOLUENE, *m*-CRESOL)

$$\lambda = A[1 + B(1 - T_r)^{1/3} + C(1 - T_r)^{2/3} + D(1 - T_r)]$$

where

λ = thermal conductivity at saturation pressure (mW/m K)

$T_r = T/T_c$, T = temperature (K)

$T_c = 705.75$ K

$A = 88.0$, $B = 3.0$, $C = -6.5$, $D = 4.7$

T K	λ mW/m K	T K	λ mW/m K	t °C	λ mW/m K	t °C	λ mW/m K
280	(152.)	470	(134.0)	10	(152.)	200	(133.8)
290	(151.0)	480	(133.)	20	150.6	210	(133.)
300	149.8	490	(133.)	30	149.5	220	(133.)
310	148.7	500	(132.)	40	148.3	230	(132.)
320	147.5	510	(132.)	50	147.2	240	(131.)
330	146.4	520	(131.)	60	146.1	250	(131.)
340	145.4	530	(131.)	70	145.0	260	(131.)
350	144.3	540	(130.)	80	144.0	270	(130.)
360	(143.3)	550	(130.)	90	(143.0)	280	(130.)
370	(142.3)	560	(130.)	100	(142.0)	290	(130.)
380	(141.3)	570	(129.)	110	(141.0)	300	(129.)
390	(140.4)	580	(129.)	120	(140.1)	310	(129.)
400	(139.4)	590	(129.)	130	(139.2)	320	(129.)
410	(138.6)	600	(129.)	140	(138.3)	330	(129.)
420	(137.7)	610	(129.)	150	(137.5)	340	(129.)
430	(136.9)	620	(129.)	160	(136.6)	350	(129.)
440	(136.1)	630	(129.)	170	(135.9)	360	(129.)
450	(135.4)	640	(129.)	180	(135.1)	370	(129.)
460	(134.6)			190	(134.4)		

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4-CH₃C₆H₄OH 4-METHYLPHENOL (4-HYDROXYTOLUENE, *p*-CRESOL)

$$\lambda = A[1 + B(1 - T_r)^{1/3} + C(1 - T_r)^{2/3} + D(1 - T_r)]$$

where

λ = thermal conductivity at saturation pressure (mW/m K)

$T_r = T/T_c$, T = temperature (K)

$T_c = 704.55$ K

$A = 86.0$, $B = 3.0$, $C = -6.5$, $D = 4.7$

T K	λ mW/m K	T K	λ mW/m K	t °C	λ mW/m K	t °C	λ mW/m K
300	(146.)	480	(130.)	30	(146.)	210	(130.)
310	(145.2)	490	(130.)	40	(144.9)	220	(129.)
320	(144.1)	500	(129.)	50	(143.8)	230	(129.)
330	(143.0)	510	(129.)	60	(142.7)	240	(128.)
340	(142.0)	520	(128.)	70	(141.7)	250	(128.)
350	(141.0)	530	(128.)	80	(140.6)	260	(128.)
360	(140.0)	540	(127.)	90	(139.6)	270	(127.)
370	(139.0)	550	(127.)	100	(138.7)	280	(127.)
380	(138.)	560	(127.)	110	(138.)	290	(127.)
390	(137.)	570	(126.)	120	(137.)	300	(126.)
400	(136.)	580	(126.)	130	(136.)	310	(126.)
410	(135.)	590	(126.)	140	(135.)	320	(126.)
420	(135.)	600	(126.)	150	(134.)	330	(126.)
430	(134.)	610	(126.)	160	(133.)	340	(126.)
440	(133.)	620	(126.)	170	(133.)	350	(126.)
450	(132.)	630	(126.)	180	(132.)	360	(126.)
460	(132.)	640	(126.)	190	(131.)	370	(126.)
470	(131.)			200	(131.)		

*MASON, H.L.

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* Single-point measurement below 300 K.