

Thermophysical properties of industrially important fluids on the saturation line: Xylenols

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THERMOPHYSICAL PROPERTIES OF INDUSTRIALLY IMPORTANT FLUIDS ON THE SATURATION LINE: XYLENOLS

CONTENTS

	Page
1. INTRODUCTION	1
2. NOTATION AND UNITS	1
3. EQUATIONS FOR PROPERTIES	2
3.1 Vapour Pressure	2
3.2 Density of the Saturated Liquid	2
3.3 Density of the Saturated Vapour	2
3.4 Specific Enthalpy of the Saturated Liquid	3
3.5 Latent Heat of Vaporisation (Specific Enthalpy of Vaporisation)	3
3.6 Specific Enthalpy of the Saturated Vapour	3
3.7 Isobaric Specific Heat Capacity of the Saturated Liquid	3
3.8 Isobaric Specific Heat Capacity of the Saturated Vapour	3
3.9 Specific Heat Capacity at Saturation of the Saturated Liquid	3
3.10 Dynamic Viscosity of the Saturated Liquid	4
3.11 Dynamic Viscosity of the Saturated Vapour	4
3.12 Thermal Conductivity of the Saturated Liquid	4
3.13 Thermal Conductivity of the Saturated Vapour	4
3.14 Surface Tension	4
4. EXPLANATION OF THE TABLES AND FIGURES	4
5. DERIVATION	5
6. TABLES	7
TABLE 6.1 Physical constants of 2,3-xylenol and constants for Equations (3.1) to (3.14)	7
TABLE 6.2 Thermophysical properties of 2,3-xylenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.1	8
TABLE 6.3 Thermophysical properties of 2,3-xylenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.1	10
TABLE 6.4 Physical constants of 2,4-xylenol and constants for Equations (3.1) to (3.14)	12
TABLE 6.5 Thermophysical properties of 2,4-xylenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.4	13

TABLE 6.6	Thermophysical properties of 2,4-xilenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.4	15
TABLE 6.7	Physical constants of 2,5-xilenol and constants for Equations (3.1) to (3.14)	17
TABLE 6.8	Thermophysical properties of 2,5-xilenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.7	18
TABLE 6.9	Thermophysical properties of 2,5-xilenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.7	20
TABLE 6.10	Physical constants of 2,6-xilenol and constants for Equations (3.1) to (3.14)	22
TABLE 6.11	Thermophysical properties of 2,6-xilenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.10	23
TABLE 6.12	Thermophysical properties of 2,6-xilenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.10	25
TABLE 6.13	Physical constants of 3,4-xilenol and constants for Equations (3.1) to (3.14)	27
TABLE 6.14	Thermophysical properties of 3,4-xilenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.13	28
TABLE 6.15	Thermophysical properties of 3,4-xilenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.13	30
TABLE 6.16	Physical constants of 3,5-xilenol and constants for Equations (3.1) to (3.14)	32
TABLE 6.17	Thermophysical properties of 3,5-xilenol on the saturation line calculated from Equations (3.1) to (3.6) and the constants in Table 6.16	33
TABLE 6.18	Thermophysical properties of 3,5-xilenol on the saturation line calculated from Equations (3.7) to (3.14) and the constants in Table 6.16	35
7.	FIGURES	37
FIGURE 1	VAPOUR PRESSURE OF 2,5–XYLENOL	37
FIGURE 2	SATURATION DENSITIES OF 2,5–XYLENOL	37
FIGURE 3	SATURATION SPECIFIC ENTHALPIES OF 2,5–XYLENOL AND SPECIFIC ENTHALPY OF VAPORISATION	38
FIGURE 4	SATURATION SPECIFIC HEAT CAPACITIES OF 2,5–XYLENOL	38
FIGURE 5	SATURATION VISCOSITIES OF 2,5–XYLENOL	39

FIGURE 6	SATURATION THERMAL CONDUCTIVITIES OF 2,5–XYLENOL	39
FIGURE 7	SURFACE TENSION OF 2,5–XYLENOL	40
APPENDIX A	CONVERSION FACTORS	41
APPENDIX B		42
B1.	SPECIFIC HEAT CAPACITIES OF SATURATED LIQUIDS AND VAPOURS	42

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THERMOPHYSICAL PROPERTIES OF INDUSTRIALLY IMPORTANT FLUIDS ON THE SATURATION LINE: XYLENOLS

1. INTRODUCTION

This Item, which is one of a series concerned with the thermophysical properties of industrially important fluids, gives equations representing the thermophysical properties of 2,3-xyleneol, 2,4-xyleneol, 2,5-xyleneol, 2,6-xyleneol, 3,4-xyleneol and 3,5-xyleneol on the saturation line, together with tabulated values calculated from the equations.

The data on which the recommended values of the fluid properties are based are considered to be the best available and the range covered for the saturation line properties is from the melting temperature to within at least 75 kelvin of the critical temperature.

All quantities are expressed in SI units or their multiples (see Section 2) but, for users who require them in other units, conversion factors are provided in Appendix A. Equations representing the fluid properties are given in Section 3 and Section 4 gives an explanation of the Tables and Figures in the Data Item.

2. NOTATION AND UNITS

b_1, b_2, b_3, b_4, b_5	constants in Equations (3.1) to (3.14)	*
c	specific heat capacity	kJ/kg K
h	specific enthalpy	kJ/kg
M	molecular weight (relative molecular mass)	—
p	vapour pressure	kPa
T	kelvin temperature	K
t	Celsius temperature, $(T - 273.15)$	°C
u	specific internal energy	kJ/kg
V	molar volume	cm ³ /mol
v	specific volume, $v = 1/\rho$	m ³ /kg
η	dynamic viscosity	mN s/m ² or $\mu\text{N s/m}^2$
θ	temperature dependent variable in Equation (3.10)	—
λ	thermal conductivity	mW/m K
ρ	density	kg/m ³
σ	surface tension	mN/m
ω	acentric factor	—

* The constants b are dimensionless except for the following: Equations (3.4) and (3.6), kJ/kg (all); Equations (3.7) and (3.9), kJ/kg K (all); Equation (3.8), kJ/kg K (b_1); Equation (3.10), K (b_3), mN s/m² (b_4); Equation (3.11), $\mu\text{N s/m}^2$ ($\exp(b_1)$); Equations (3.12) and (3.13), mW/m K (b_1 and $\exp(b_1)$ respectively); Equation (3.14), mN/m (b_1).

State descriptors

(g)	value for gas or saturated vapour
(l)	value for saturated liquid
Δ	denotes property difference between two states

Subscripts

b	value at normal boiling point
c	value at critical point
m	value at normal melting point
p	value at constant pressure
r	denotes reduced quantity, <i>e.g.</i> $T_r = T/T_c$
sat	value at saturation (defined in Appendix B, Section B1)
v	value at constant volume
vap	denotes evaporation.

3. EQUATIONS FOR PROPERTIES

3.1 Vapour Pressure

Data for the vapour pressure are represented by Equation (3.1).

$$\log_e \left(\frac{p}{p_c} \right) = \frac{1}{T_r} [b_1(1 - T_r) + b_2(1 - T_r)^{3/2} + b_3(1 - T_r)^3 + b_4(1 - T_r)^6]. \quad (3.1)$$

3.2 Density of the Saturated Liquid

Data for the density of the saturated liquid are represented by Equation (3.2).

$$\log_e \left(\frac{\rho(l)}{\rho_c} \right) = b_1(1 - T_r)^{1/3} + b_2(1 - T_r)^{2/3} + b_3(1 - T_r) + b_4(1 - T_r)^{4/3}. \quad (3.2)$$

3.3 Density of the Saturated Vapour

Data for the density of the saturated vapour are represented by Equation (3.3).

$$\log_e \left(\frac{\rho(g)}{\rho_c} \right) = b_1 \left(\frac{1}{T_r} - 1 \right)^{1/3} + b_2 \left(\frac{1}{T_r} - 1 \right)^{2/3} + b_3 \left(\frac{1}{T_r} - 1 \right) + b_4 \left(\frac{1}{T_r} - 1 \right)^{4/3} + b_5 \left(\frac{1}{T_r} - 1 \right)^{5/3}. \quad (3.3)$$

3.4 Specific Enthalpy of the Saturated Liquid

Data for the specific enthalpy of the saturated liquid are represented by Equation (3.4).

$$h(l) = b_1(1 - T_r)^{1/3} + b_2(1 - T_r)^{2/3} + b_3(1 - T_r) + b_4(1 - T_r)^{4/3} + b_5(1 - T_r)^{5/3} . \quad (3.4)$$

3.5 Latent Heat of Vaporisation (Specific Enthalpy of Vaporisation)

Data for the latent heat of vaporisation are represented by Equation (3.5).

$$\Delta_{\text{vap}} h = h(g) - h(l) . \quad (3.5)$$

3.6 Specific Enthalpy of the Saturated Vapour

Data for the specific enthalpy of the saturated vapour are represented by Equation (3.6).

$$h(g) = b_1(1 - T_r)^{1/3} + b_2(1 - T_r)^{2/3} + b_3(1 - T_r) + b_4(1 - T_r)^{4/3} + b_5(1 - T_r)^{5/3} . \quad (3.6)$$

3.7 Isobaric Specific Heat Capacity of the Saturated Liquid

Data for the isobaric specific heat capacity of the saturated liquid are represented by Equation (3.7).

$$c_p(l) = b_1(1 - T_r)^{-2/3} + b_2(1 - T_r)^{-1/3} + b_3(1 - T_r) + b_4(1 - T_r)^{2/3} . \quad (3.7)$$

The significance of $c_p(l)$ as a representation of specific heat capacity is fully explained in Appendix B, Section B1.

3.8 Isobaric Specific Heat Capacity of the Saturated Vapour

Data for the isobaric specific heat capacity of the saturated vapour are represented by Equation (3.8).

$$c_p(g) = b_1[1 + b_2(1 - T_r)^{-2/3} + b_3(1 - T_r)^{-1/3} + b_4(1 - T_r)^{1/3} + b_5(1 - T_r)^{2/3}] . \quad (3.8)$$

The significance of $c_p(g)$ as a representation of specific heat capacity is fully explained in Appendix B, Section B1.

3.9 Specific Heat Capacity at Saturation of the Saturated Liquid

Data for the specific heat capacity at saturation of the saturated liquid are represented by Equation (3.9).

$$c_{\text{sat}}(l) = b_1(1 - T_r)^{-2/3} + b_2(1 - T_r)^{-1/3} + b_3(1 - T_r) + b_4(1 - T_r)^{2/3} . \quad (3.9)$$

The significance of $c_{\text{sat}}(l)$ as a representation of specific heat capacity is fully explained in Appendix B, Section B1.

3.10 Dynamic Viscosity of the Saturated Liquid

Data for the dynamic viscosity of the saturated liquid are represented by Equation (3.10).

$$\eta(l) = b_4 \exp[b_1(\theta - 1)^{1/3} + b_2(\theta - 1)^{4/3}] \quad (3.10)$$

where $\theta = (T_c - b_3)/(T - b_3)$.

3.11 Dynamic Viscosity of the Saturated Vapour

Data for the dynamic viscosity of the saturated vapour are represented by Equation (3.11).

$$\log_e \eta(g) = b_1 + b_2 \left(\frac{1}{T_r} - 1 \right)^{1/3} + b_3 \left(\frac{1}{T_r} - 1 \right)^{4/3}. \quad (3.11)$$

3.12 Thermal Conductivity of the Saturated Liquid

Data for the thermal conductivity of the saturated liquid are represented by Equation (3.12).

$$\lambda(l) = b_1 [1 + b_2(1 - T_r)^{1/3} + b_3(1 - T_r)^{2/3} + b_4(1 - T_r)]. \quad (3.12)$$

3.13 Thermal Conductivity of the Saturated Vapour

Data for the thermal conductivity of the saturated vapour are represented by Equation (3.13).

$$\log_e \lambda(g) = b_1 + b_2(1 - T_r)^{-2/3} + b_3(1 - T_r)^{-1/3} + b_4(1 - T_r)^{1/3} + b_5(1 - T_r)^{2/3}. \quad (3.13)$$

3.14 Surface Tension

Data for surface tension are represented by Equation (3.14).

$$\sigma = b_1(1 - T_r)^{b_2} [1 + b_3(1 - T_r)]. \quad (3.14)$$

4. EXPLANATION OF THE TABLES AND FIGURES

Tables 6.1, 6.4, 6.7, 6.10, 6.13 and 6.16 provide values of the physical constants for 2,3-xyleneol, 2,4-xyleneol, 2,5-xyleneol, 2,6-xyleneol, 3,4-xyleneol and 3,5-xyleneol respectively and constants for use in the equations given in Section 3, that represent the fluid properties in the SI units* of the Notation, Section 2. Although for 3,5-xyleneol the saturated liquid and vapour densities tend to the same value as the critical point is approached, only the saturated liquid density curve, Equation (3.2) displays physically realistic behaviour near the critical point. At some value of reduced temperature below unity, the saturated vapour density values calculated from Equation (3.3) exceed the critical value. Also for all the xyleneols, the saturated liquid enthalpy values calculated from Equation (3.4) pass through a physically unrealistic maximum so that although the liquid and vapour enthalpies tend to the same value, the slope of the saturated liquid enthalpy curve tends to $-\infty$ at the critical temperature, not ∞ as required.

* Appendix A gives conversion factors to other units.

Modern theory requires the isobaric heat capacity, viscosity and thermal conductivity to tend to infinity as the critical point is approached; this theoretical limit has been included where appropriate in Tables 6.3, 6.6, 6.9, 6.12 and 6.15. However, for all the xylenols, Equations (3.8), (3.10), (3.11), (3.12), (3.13) do not conform with theory in this respect; Equation (3.8) approaches $-\infty$, Equations (3.10), (3.11), (3.12) approach a finite value and Equation (3.13) goes to zero at the critical temperature. Although the remaining equations, Equations (3.1), (3.2), (3.5), (3.6), (3.7), (3.9), (3.14) extrapolate in a physically realistic manner, users should not extrapolate any of the equations in Section 3 outside the temperature limits specified in Tables 6.1, 6.4, 6.7, 6.10, 6.13 and 6.16.

The variation with temperature of all the fluid properties for 2,5-xyleneol is shown in Figures 1 to 7. The dashed lines show the extrapolated behaviour of some of these equations between the upper temperature limits in Table 6.7 and the critical temperature. The corresponding variations of fluid properties for the other xylenols are not plotted since they are very similar in form to those for 2,5-xyleneol.

The values derived from the equations applying on the saturation line are presented in: Tables 6.2 and 6.3 (2,3-xyleneol); Tables 6.5 and 6.6 (2,4-xyleneol); Tables 6.8 and 6.9 (2,5-xyleneol); Tables 6.11 and 6.12 (2,6-xyleneol); Tables 6.14 and 6.15 (3,4-xyleneol) and Tables 6.17 and 6.18 (3,5-xyleneol). The temperature range covered is from the melting temperature to approximately $T_r = 0.90$, except for Equation (3.1) which is valid to the critical temperature and Equations (3.2), (3.3), (3.4), (3.5), (3.6), (3.10), (3.11), (3.13) and (3.14), which are valid to approximately $T_r = 0.98$.

The specific enthalpies of vaporisation in column 7 of Tables 6.2, 6.5, 6.8, 6.11 and 6.14 were calculated directly from Equation (3.5) with subsequent rounding to the desired number of significant figures. Small differences, usually in the last figure may occur therefore, between these values and those obtained by subtraction of the specific enthalpies in column 5 from those in column 6, since the values generated thereby are the differences between two rounded numbers values generated closely.

The data used in developing the constants for the equations are those considered to be the best available and the equations themselves introduce no significant fitting errors. For some properties, however, where experimental data are few or lacking it has been necessary to estimate values and these are indicated in the Tables by the use of parentheses.

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The Derivation lists selected sources that have assisted in the preparation of this Data Item.

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6. TABLES

$C_8H_{10}O$ 2,3-XYLENOL CAS Reg. No: 526-75-0

**TABLE 6.1 Physical constants of 2,3-xyleneol and constants
for Equations (3.1) to (3.14)**

Physical Constants	Symbol	Value
Molecular Weight	M	122.168
Critical Temperature	T_c	722.8 K (449.65 °C)
Critical Pressure	p_c	4625.0 kPa
Critical Density	ρ_c	340. kg/m ³
Critical Molar Volume	V_c	359. cm ³ /mol
Normal Boiling Temperature	T_b	490.07 K (216.92 °C)
Normal Melting Temperature	T_m	345.95 K (72.80 °C)
Acentric Factor	ω	0.495

Constants used in Equations (3.1) to (3.14)

Property	Equation in Section 3	b_1	b_2	b_3	b_4	b_5	Range of Applicability °C
p	(3.1)	-10.1112	5.17092	-8.36627	-0.43918	-	73 to 440
$\rho(l)$	(3.2)	1.49489	-0.166712	0.179483	-0.308647	-	73 to 435
$\rho(g)$	(3.3)	-1.22633	-7.22946	6.864	-4.94673	-2.61433	73 to 435
$h(l)$	(3.4)	6922.716	-31367.3	64233.1	-66658.3	26085.7	73 to 435
$h(g)$	(3.6)	7008.47	-26953.9	51213.7	-51373.7	19965.	73 to 435
$c_p(l)$	(3.7)	0.661808	-1.01239	-14.9242	15.8041	-	73 to 380
$c_p(g)$	(3.8)	-16.1422	0.0410746	-0.379477	-1.557	0.876587	73 to 380
$c_{sat}(l)$	(3.9)	0.568561	-0.829643	-14.7742	15.5465	-	73 to 380
$\eta(l)$	(3.10)	2.2571	0.1789	231.23	0.034	-	73 to 435
$\eta(g)$	(3.11)	3.2151	-1.12422	-0.0794695	-	-	73 to 435
$\lambda(l)$	(3.12)	84.099	3.5	-8.1	6.	-	73 to 380
$\lambda(g)$	(3.13)	-10.8715	-0.381368	3.92577	24.5173	-16.2296	73 to 430
σ	(3.14)	60.61	1.1351	0	-	-	73 to 435

TABLE 6.2
Thermophysical properties of 2,3-xylenol on the saturation line
calculated from Equations (3.1) to (3.6) and the constants in Table 6.1

t °C	p kPa	$\rho(l)$ kg/m ³	$\rho(g)$ kg/m ³	$h(l)$ kJ/kg	$h(g)$ kJ/kg	$\Delta_{vap}h$ kJ/kg
72.80	0.36654	(980.6)	(0.015468)	(-420.)	(66.9)	(487.)
75	0.41814	(979.2)	(0.017554)	(-415.)	(70.2)	(485.)
80	0.55979	(975.9)	(0.023220)	(-404.)	(77.8)	(482.)
85	0.74183	(972.6)	(0.030393)	(-393.)	(85.5)	(479.)
90	0.97355	(969.2)	(0.039390)	(-382.)	(93.2)	(475.)
95	1.2658	(965.8)	(0.050569)	(-371.)	(101.)	(472.)
100	1.6313	(962.3)	(0.064344)	(-360.)	(109.)	(469.)
105	2.0846	(958.8)	(0.081177)	(-348.)	(117.)	(465.)
110	2.6423	(955.2)	(0.10159)	(-337.)	(125.)	(462.)
115	3.3232	(951.6)	(0.12616)	(-325.)	(133.)	(458.)
120	4.1488	(948.0)	(0.15554)	(-313.)	(142.)	(455.)
125	5.1426	(944.3)	(0.19042)	(-302.)	(150.)	(452.)
130	6.3314	(940.6)	(0.23159)	(-290.)	(158.)	(448.)
135	7.7442	(936.8)	(0.27988)	(-278.)	(167.)	(445.)
140	9.4132	(932.9)	(0.33621)	(-266.)	(175.)	(441.)
145	11.374	(929.0)	(0.40157)	(-254.)	(184.)	(438.)
150	13.663	(925.1)	(0.47701)	(-242.)	(193.)	(434.)
155	16.324	(921.1)	(0.56368)	(-230.)	(201.)	(431.)
160	19.400	(917.1)	(0.66277)	(-217.)	(210.)	(427.)
165	22.939	(913.0)	(0.77558)	(-205.)	(219.)	(424.)
170	26.992	(908.8)	(0.90346)	(-193.)	(228.)	(420.)
175	31.613	(904.6)	(1.0479)	(-180.)	(237.)	(417.)
180	36.860	(900.3)	(1.2103)	(-168.)	(246.)	(413.)
185	42.792	(896.0)	(1.3924)	(-155.)	(255.)	(410.)
190	49.475	(891.6)	(1.5958)	(-142.)	(264.)	(406.)
195	56.974	(887.2)	(1.8223)	(-130.)	(273.)	(403.)
200	65.361	(882.6)	(2.0737)	(-117.)	(282.)	(399.)
205	74.708	(878.1)	(2.3519)	(-104.)	(292.)	(396.)
210	85.091	(873.4)	(2.6590)	(-91.4)	(301.)	(392.)
215	96.591	(868.7)	(2.9972)	(-78.6)	(310.)	(389.)
216.92	101.325	(866.9)	(3.1357)	(-73.7)	(314.)	(387.)
220	109.29	(863.9)	(3.3685)	(-65.7)	(319.)	(385.)
225	123.27	(859.1)	(3.7753)	(-52.9)	(329.)	(382.)
230	138.63	(854.2)	(4.2200)	(-40.0)	(338.)	(378.)
235	155.45	(849.2)	(4.7052)	(-27.0)	(348.)	(375.)
240	173.83	(844.1)	(5.2334)	(-14.1)	(357.)	(371.)
245	193.87	(838.9)	(5.8075)	(-1.10)	(366.)	(368.)
250	215.67	(833.7)	(6.4303)	(11.9)	(376.)	(364.)
255	239.34	(828.4)	(7.1050)	(24.9)	(385.)	(360.)
260	264.97	(822.9)	(7.8347)	(37.9)	(395.)	(357.)
265	292.70	(817.4)	(8.6229)	(50.9)	(404.)	(353.)
270	322.62	(811.8)	(9.4731)	(63.9)	(414.)	(350.)
275	354.87	(806.2)	(10.389)	(77.0)	(423.)	(346.)
280	389.56	(800.4)	(11.376)	(90.0)	(433.)	(343.)
285	(426.83)	(794.5)	(12.436)	(103.)	(442.)	(339.)
290	(466.82)	(788.5)	(13.576)	(116.)	(452.)	(336.)

TABLE 6.2 (continued)
Thermophysical properties of 2,3-xylenol on the saturation line
calculated from Equations (3.1) to (3.6) and the constants in Table 6.1

t °C	p kPa	$\rho(l)$ kg/m ³	$\rho(g)$ kg/m ³	$h(l)$ kJ/kg	$h(g)$ kJ/kg	$\Delta_{\text{vap}} h$ kJ/kg
295	(509.65)	(782.4)	(14.800)	(129.)	(461.)	(332.)
300	(555.48)	(776.1)	(16.113)	(142.)	(471.)	(328.)
305	(604.47)	(769.8)	(17.522)	(155.)	(480.)	(325.)
310	(656.77)	(763.3)	(19.033)	(168.)	(489.)	(321.)
315	(712.55)	(756.7)	(20.653)	(181.)	(499.)	(317.)
320	(771.99)	(749.9)	(22.390)	(194.)	(508.)	(314.)
325	(835.28)	(743.0)	(24.252)	(207.)	(517.)	(310.)
330	(902.60)	(735.9)	(26.249)	(220.)	(527.)	(306.)
335	(974.18)	(728.7)	(28.392)	(234.)	(536.)	(302.)
340	(1050.2)	(721.3)	(30.692)	(247.)	(545.)	(299.)
345	(1131.0)	(713.7)	(33.163)	(260.)	(554.)	(295.)
350	(1216.7)	(705.9)	(35.820)	(273.)	(564.)	(291.)
355	(1307.7)	(697.9)	(38.681)	(286.)	(573.)	(286.)
360	(1404.1)	(689.6)	(41.765)	(300.)	(582.)	(282.)
365	(1506.4)	(681.1)	(45.097)	(313.)	(591.)	(278.)
370	(1614.9)	(672.4)	(48.703)	(326.)	(600.)	(273.)
375	(1729.9)	(663.3)	(52.615)	(340.)	(609.)	(269.)
380	(1851.8)	(653.9)	(56.872)	(354.)	(618.)	(264.)
385	(1981.0)	(644.1)	(61.521)	(368.)	(626.)	(258.)
390	(2118.0)	(633.9)	(66.618)	(382.)	(635.)	(253.)
395	(2263.3)	(623.3)	(72.233)	(397.)	(644.)	(247.)
400	(2417.5)	(612.1)	(78.454)	(412.)	(652.)	(241.)
405	(2581.2)	(600.3)	(85.397)	(427.)	(660.)	(233.)
410	(2755.1)	(587.7)	(93.212)	(443.)	(668.)	(226.)
415	(2939.9)	(574.3)	(102.10)	(459.)	(676.)	(217.)
420	(3136.7)	(559.9)	(112.36)	(476.)	(683.)	(207.)
425	(3346.3)	(544.0)	(124.42)	(493.)	(688.)	(195.)
430	(3570.0)	(526.2)	(138.96)	(511.)	(692.)	(181.)
435	(3809.3)	(505.8)	(157.17)	(529.)	(691.)	(163.)
440	(4066.2)					
445						
449.65	(4625.0)	(340.)	(340.)	-	-	0