A. Θερμοφυσικές ιδιότητες ουσιών (DIPPR,1997)

V. KEY FOR EQUATION FORMS

34

Number	Equation
100	$Y = A + BT + CT^2 + DT^3 + ET^4$
101	$Y = \exp\left[A + \frac{B}{T} + C\,\ell nT + DT^E\right]$
102	$Y = \frac{AT^B}{1 + \frac{C}{T} + \frac{D}{T^2}}$
103*	$Y = A + B \exp\left[\frac{-C}{T^D}\right]$
104	$Y = A + \frac{B}{T} + \frac{C}{T^3} + \frac{D}{T^8} + \frac{E}{T^9}$
105	$Y = A/B^{(1+(1-T/C)^D)}$
106	$Y = A(1 - T_r)^{(B+CT_r+DT_r^2+ET_r^3)}$
107**	$Y = A + B\,[(C/T)/\sinh(C/T)]^2 + D\,[(E/T)/\cosh(E/T)]^2$
114	$Y = \frac{A^2}{t} + B - 2ACt - ADt^2 - \frac{C^2t^3}{3} - \frac{CDt^4}{2} - \frac{D^2t^5}{5}$ where $t = (1 - T_r)$

Εξίσωση για cp

Εξίσωση για πυκνότητα

**Integration of Equation 107

$$C_p^* = A + B\left[\left(\frac{C}{T}\right)/\sinh\left(\frac{C}{T}\right)\right]^2 + D\left[\left(\frac{E}{T}\right)/\cosh\left(\frac{E}{T}\right)\right]^2$$

$$H^* = AT + BC\coth(C/T) - DE\tanh\left(\frac{E}{T}\right) + HCON$$

$$S^* = A\,\ell n\,T + B\left[\left(\frac{C}{T}\right)\coth\left(\frac{C}{T}\right) - \ell n\sinh\left(\frac{C}{T}\right)\right] - D\left[\frac{E}{T}\tanh\left(\frac{E}{T}\right) - \ell n\cosh\left(\frac{E}{T}\right)\right] + SCON$$

HCON and SCON are integration constants

* Not used currently.

Y = the property in units shown on page III-1

T = temperature in kelvins; T_r = reduced temperature

A, B, C, D, E = Specific constants for compound and property listed in equation coefficient tables

Rev. 1994

Ισοπροπανόλη

PROPERTY CONSTANTS

Chemical Abstracts Name: 2-PROPANOL — C3H8O
IUPAC NAME: 2-PROPANOL — ISOPROPANOL
Synonyms: DIMETHYL CARBINOL; ISOHOL; 1-METHYLETHYL ALCOHOL; PROPANE, 2-HYDROXY-; PROPAN-2-OL; Hsec-PROPYL ALCOHOL; 2-HYDROXYPROPANE; ISOPROPYL ALCOHOL; PETROHOL; sec-PROPANOL; n-PROPAN-2-OL
Chemical Abstracts Number: 67-63-0 Structural Formula: CH3CHOHCH3

PROPERTY	UNITS	VALUE	NOTE	QUAL CODE	ACCEPTED REFERENCE(S)	REJECTED REFERENCE(S)
*Molecular Weight	kg/kmol	60.096	1		1	
Critical Temperature	K	508.31		XE2	30 22 3	
Critical Pressure	Pa	4.7643E+06		XE3	30 3 22	
Critical Volume	m**3/kmol	0.22013		XE4	30 22 533	
Crit Compress Factor		0.248		D	3	
Melting Point	K	185.28	2	P 2	PS 30 3	
Triple Pt Temperature	K	185.28		XU2	472 305	
Triple Pt Pressure	Pa	3.2000E-02		P 3P	PS	
Normal Boiling Point	K	355.41		XE3	30 3 22	
Liq Molar Volume	m**3/kmol	0.076784		X 1P	PS	
IG Heat of Formation	J/kmol	-2.7242E+08		XE2	30 3	
IG Gibbs of Formation	J/kmol	-1.7339E+08		XE1	30 3	
IG Absolute Entropy	J/kmol*K	3.0991E+05		XE1	30 3 2498	
Heat Fusion at Melt Pt	J/kmol	5.4099E+06		XE2	3 305 2865	363
Stand Net Heat of Comb	J/kmol	-1.8300E+09		XE2Y	400	
Acentric Factor		0.6689		D	PS 22	11
Radius of Gyration	m	2.8070E-10		D 3	1112 11 12	
Solubility Parameter	(J/m**3)**.5	2.3575E+04		D 3	PS	
Dipole Moment	C*m	5.5372E-30		XE1Z	25 39 4	
van der Waals Volume	m**3/kmol	0.04216		D 2	72	
van der Waals Area	m**2/kmol	6.2700E+08		D 2	72	
Refractive Index		1.3752		XE1	30 3 8	
Flash Point	K	284.82		XU0	256 39	
Flammability Limits	vol %	2.0 TO 12.0		XU0	256	
Autoignition Temp	K	672.04		XU0	256	

Issue Date: JULY 1981 Revision Date: AUG. 1987

NOTES: 1. Acutely toxic chemical identified by EPA. C & EN, p. 20, January 6, 1986.
2. Estimated to be equal to the triple point temperature.

EQUATION COEFFICIENTS

Chemical Abstracts Name: 2-PROPANOL — C3H8O ISOPROPANOL

Property	NTE	EQN	Q	COEFFICIENTS A	B	C	D	E
Solid Density Only one value available (185.28, 1.7100E+01)	1	100	6	1.7100E+01				
Liquid Density Min(185.28, 1.4656E+01) Max(508.31, 4.4570E+00)		105	2	1.1800E+00	2.6475E-01	5.0831E+02	2.4300E-01	
Vapor Pressure Min(185.28, 3.2000E-02) Max(508.31, 4.7673E+06)	2	101	3	9.2935E+01	-8.1771E+03	-1.0031E+01	3.9988E-06	2.0000E+00
Heat of Vaporization Min(185.28, 5.2121E+07) Max(508.31, 0.0000E+00)	3	106	3	5.6980E+07	8.7000E-02	3.0070E-01		
Solid Heat Capacity Min(12.00, 1.8460E+03) Max(176.66, 9.1821E+04)		100	3	-8.5000E+03	8.7600E+02	-8.1000E-01	-3.0250E-02	1.4130E-04
Liquid Heat Capacity Min(188.32, 1.1277E+05) Max(463.15, 2.7174E+05)		100	3	4.6640E+05	-4.1086E+03	1.4506E+01	-1.4126E-02	
*Ideal Gas Heat Capacity Min(100.00, 4.8262E+04) Max(1500.00, 2.1652E+05)		107	3	4.7460E+04	1.9350E+05	1.1240E+03	9.3800E+04	4.6000E+02
Second Virial Coefficient Min(279.58,-4.8942E+00) Max(2541.60, 2.5100E-02)		104	4	3.0200E-02	-6.2900E+00	-4.3100E+07	1.9860E+20	-8.6100E+22
Liquid Viscosity Min(187.35, 3.0037E-01) Max(354.45, 5.1389E-04)		101	5	-8.2300E+00	2.2822E+03	-9.8495E-01		
Vapor Viscosity Min(200.00, 4.8683E-06) Max(1000.00, 2.5019E-05)		102	5	1.9930E-07	7.2330E-01	1.7800E+02		
Liq Thermal Conductivity Min(185.28, 1.6069E-01) Max(410.00, 1.0950E-01)		100	3	2.0290E-01	-2.2780E-04			
Vap Thermal Conductivity Min(355.41, 2.2388E-02) Max(450.00, 3.2427E-02)		102	3	-8.0642E+01	-1.4549E+00	-6.0442E+02		
Surface Tension Min(273.15, 2.2894E-02) Max(355.41, 1.6387E-02)	4	100	2	3.8180E-02	-3.8180E-05	-6.5100E-08		

Issue Date: JULY 1981 Revision Date: AUG. 1987

NOTES: 1. Estimated by Project Staff from liquid density at the triple point.
2. Data predicted by Riedel's method used in regression.
3. Data calculated from Clapeyron equation used in regression.
4. Data regressed with equation 100 because regression with equation 106 produces B coefficient less than 1.0 while theoretical universal constant should be 1.2. (see ref. #1008).

kmol/m^3

J/(kmol K)

Μεθανόλη

PROPERTY CONSTANTS

Chemical Abstracts Name: METHANOL — CH4O METHANOL
IUPAC NAME: METHANOL
Synonyms: CARBINOL; COLONIAL SPIRIT; COLUMBIAN SPIRIT; HYDROXYMETHANE; METHYL ALCOHOL; METHYL HYDROXIDE; MONOHYDROXYMETHANE; WOOD ALCOHOL; WOOD NAPHTHA; WOOD SPIRIT
Chemical Abstracts Number: 67-56-1 Structural Formula: CH3OH

PROPERTY	UNITS	VALUE	NOTE	QUAL CODE	ACCEPTED REFERENCE(S)	REJECTED REFERENCE(S)
Molecular Weight	kg/kmol	32.042	1		1	
Critical Temperature	K	512.64		XE2	3843 3 4680	
Critical Pressure	Pa	8.0970E+06		XE3	3843 3 38	
Critical Volume	m**3/kmol	0.11800		XE4	3843 3 29	
Crit Compress Factor		0.224		D	PS 3843 3	
Melting Point	K	175.47		XE2	30 3 7	2 4
Triple Pt Temperature	K	175.47		XE2	30	
Triple Pt Pressure	Pa	1.1147E-01		P 4	PS	
Normal Boiling Point	K	337.85		XE2	30 6 3	
Liq Molar Volume	m**3/kmol	0.040581		X 2	PS	
IG Heat of Formation	J/kmol	-2.0094E+08		XE2	3565 30 3	
IG Gibbs of Formation	J/kmol	-1.6232E+08	2	D 2	PS 1511 30	
IG Absolute Entropy	J/kmol**K	2.3988E+05		XE2	3565 15 3	
Heat Fusion at Melt Pt	J/kmol	3.2150E+06		XE1Z	2865 30	29 382
Stand Net Heat of Comb	J/kmol	-6.3820E+08	3	P 2	PS 400	
Acentric Factor		0.5640		D	PS 11 12	
Radius of Gyration	m	1.5520E-10		D 3	1112 11 12	
Solubility Parameter	(J/m**3)**.5	2.9590E+04		D 3	PS	
Dipole Moment	C*m	5.6700E-30		XE2Z	25	
van der Waals Volume	m**3/kmol	0.02171		D 2	72	
van der Waals Area	m**2/kmol	3.5800E+08		D 2	72	
Refractive Index		1.3265		XE1	3 39 1492	
Flash Point	K	284.00		XU0	256	
Flammability Limits	vol %	7.3 TO 36.0	4	XU0	256	
Autoignition Temp	K	737.00		XU0	256	

Issue Date: JULY 1981 Revision Date: AUG. 1994

NOTES:
1. Acutely toxic chemical identified by EPA. C & EN, p. 20, January 6, 1986.
2. Calculated from the enthalpy of formation and the absolute entropy.
3. Value derived from enthalpy of formation.
4. WARNING: FLAMMABILITY LIMITS ARE DETERMINED AT 298 K AND 1 ATMOSPHERE. HIGHER TEMPERATURES AND/OR HIGHER PRESSURES WILL LOWER THE LOWER LIMIT AND RAISE THE UPPER LIMIT.

EQUATION COEFFICIENTS

Chemical Abstracts Name: METHANOL — CH4O METHANOL

Property	NTE	EQN	Q	COEFFICIENTS A	B	C	D	E
Solid Density Only one value available (163.15, 3.0585E+01)		100	3	3.0585E+01				
Liquid Density Min(175.47, 2.7912E+01) Max(512.64, 8.5214E+00)		105	2	2.2880E+00	2.6850E-01	5.1264E+02	2.4530E-01	
Vapor Pressure Min(175.47, 1.1147E-01) Max(512.64, 8.1402E+06)		101	2	8.1768E+01	-6.8760E+03	-8.7078E+00	7.1926E-06	2.0000E+00
Heat of Vaporization Min(175.47, 4.4900E+07) Max(512.64, 0.0000E+00)		106	3	5.2390E+07	3.6820E-01			
Solid Heat Capacity Min(25.00, 8.1982E+03) Max(150.00, 5.7752E+04)	1	100	3	-1.2706E+04	9.5878E+02	-5.2332E+00	1.3152E-02	
Liquid Heat Capacity Min(175.47, 7.1117E+04) Max(400.00, 1.1097E+05)		100	2	1.0580E+05	-3.6223E+02	9.3790E-01		
Ideal Gas Heat Capacity Min(200.00, 3.9802E+04) Max(1500.00, 1.0533E+05)	2	107	2	3.9252E+04	8.7900E+04	1.9165E+03	5.3654E+04	8.9670E+02
Second Virial Coefficient Min(298.15,-2.0770E+00) Max(1500.00,-2.7019E-03)		104	4	1.3000E-02	-1.4400E+01	-2.0600E+07	7.6000E+19	-4.6200E+22
Liquid Viscosity Min(175.47, 1.1928E-02) Max(337.85, 3.4423E-04)		101	4	-2.5317E+01	1.7892E+03	2.0690E+00		
Vapor Viscosity Min(240.00, 7.5232E-06) Max(1000.00, 3.1281E-05)		102	5	3.0663E-07	6.9655E-01	2.0500E+02		
Liq Thermal Conductivity Min(175.47, 2.3439E-01) Max(337.85, 1.8876E-01)		100	3	2.8370E-01	-2.8100E-04			
Vap Thermal Conductivity Min(273.00, 1.3652E-02) Max(1000.00, 1.3927E-01)		102	4	-7.7630E+00	1.0279E+00	-7.4360E+07	6.7700E+09	
Surface Tension Min(273.10, 2.4138E-02) Max(503.15, 8.0358E-04)	3	100	2	3.5130E-02	-7.0400E-06	-1.2160E-07		

kmol/m^3

J/(kmol K)

Issue Date: JULY 1981 Revision Date: AUG. 1989

NOTES:
1. Coefficients are for Crystal II; for Crystal I in the range 157.35 K to 175.61 K use the coefficients: A = 3.3425E+05, B = -3.7493E+03, C = 1.2214E+01. The transition point is at 157.4 K with heat of transition of 645600 J/kmol. (Ref. 383)
2. In the temperature range 50 K to 200 K use equation 100 with A = 3.0270E+04, B = 8.4640E+01, C = -1.8800E-01.
3. Data regressed with equation 100 because regression with equation 106 produces B coefficient less than 1.0 while theoretical universal constant should be 1.2. (see ref. 1008).