

Predict2000 Plus

Compound's T Correlated Parameters in DB

File Help

All Temperature Correlated Parameters and Sources Currently Stored in the Database for:

ETHANOL C2H6O Delete Property

Property	Liquid Density	Free Energy of Form	Heat of Form	Heat of Vap
Units	kmol/m ³	J/kmol	J/kmol	J/kmol
Equation No.	104	101	101	102
Source	SystemDB	SystemDB	SystemDB	SystemDB
Date Entered	01.26.01	01.26.01	01.26.01	01.26.01
Reference	1	1	1	1
Tmin K	159,05	298	298	300
Tmax K	516,25	1000	1000	516,25
A	5,767505911	-236100000	-216960000	43122000
B	0,26395	219040	-69572	516,25
C	516,25	25,659	31,744	0,079
D	0,2367	0	0	0
E	0	0	0	0

All Compound's Properties in DB

File Help

All Properties and Sources Currently Stored in the Database for:

ETHANOL C2H6O Delete Selected Prop.

Property	Value	Units	Source	Date Entered	Ref.
Ac	,637		SystemDB	04.13.00	1
Atoms	9,		SystemDB	04.13.00	1
DI	17,083	kmol/m ³	SystemDB	10.29.00	1
Gf	-1,6828E08	J/kmol	SystemDB	10.29.00	1
Hf	-2,3481E08	J/kmol	SystemDB	10.29.00	1
Hvb	3,94E07	J/kmol	SystemDB	10.29.00	1
MW	46,0684		SystemDB	04.13.00	1
Pc	6,384E06	pascal	SystemDB	04.13.00	1
S	282.590,	J/kmol K	SystemDB	10.29.00	1
Sf	-223.143,	J/kmol K	SystemDB	10.29.00	1
Tb	351,44	K	SystemDB	04.13.00	1
Tc	516,25	K	SystemDB	04.13.00	1
Tm	159,05	K	SystemDB	04.13.00	1
Vc	,1669	m ³ /kmol	SystemDB	04.13.00	1
Zc	,248		SystemDB	04.13.00	1

Compound Information & Point Properties

File Load Compound Update DB Help

System and User DB - Compound Information and Point Properties

Empirical Formula	C2H6O
Common Name	ETHANOL
Chemical Abstracts Name	ETHANOL
IUPAC Name	ETHANOL
Structural Formula	CH3CH2OH
CAS Number	64175

	System Database (Not Editable)	User Database (Editable)	
Molecular Weight	46.0684		
Melting Point Temperature	159.05		K
Normal Boiling Point	351.44		K
Critical Temperature	516.25		K
Critical Pressure	6.384E06		pascal
Critical Volume	.1669		m ³ /kmol
Critical Compressibility, Zc	.248		
Liquid Density (@Tb)	17.083		kmol/m ³
Heat of Vaporization (@298K)			J/kmol
Heat of Vaporization (@Tb)	3.94E07		J/kmol
Heat of Formation (@298K)	-2.3481E08		J/kmol
IG Std. Entropy (@298K)	282.590		J/(kmol K)
IG Entropy of Form (@298K)	-223.143		J/(kmol K)
IG Free Energy of Form (@298K)	-1.6828E08		J/kmol
Acentric Factor	.637		
Polarity Factor			
Reidel Factor			

Units Selection

Return Help

Default Unit Sets

SI Metric English

Temperature Units	Pressure Units	Enthalpy Units
K	pascal	J/kmol
C	bar	cal/gmol
F	lbf/in ² (psi)	BTU/lbmol
R	N/m ²	kcal/gmol
	atmosphere	kcal/kmol

Entropy/Heat Cap.	Volume Units	Density Units
J/(kmol K)	m ³ /kmol	kmol/m ³
cal/(gmol C)	mL/gmol	gmol/mL
BTU/(lbmol F)	ft ³ /lbmol	lbmol/ft ³
kcal/(kmol K)	gal/lbmol	lbmol/gal
	L/kmol	kmol/L

Surface Tension Units	Viscosity Units	Thermal Conductivity
N/m	Pa s	J/(s m K)
dyne/cm	poise	(cal cm)/(s cm ² C)
poundal/in	lbm/(s ft)	(BTU ft)/(hr ft ² F)
	g/(sec cm)	(W cm)/(cm ² C)
	lbm/(hr ft)	(BTU in)/(hr ft ² F)

Done

Reichenberg Gas Viscosity Group Contribu...

<input checked="" type="checkbox"/>	-CH3	<input type="checkbox"/>	-CHO (aldehydes)
<input checked="" type="checkbox"/>	>CH2 (nonring)	<input type="checkbox"/>	-COOH (acids)
<input type="checkbox"/>	>CH- (nonring)	<input type="checkbox"/>	-COO-(ester) or HC00-
<input type="checkbox"/>	>C< (nonring)	<input type="checkbox"/>	-NH2
<input type="checkbox"/>	=CH2	<input type="checkbox"/>	>NH (nonring)
<input type="checkbox"/>	=CH- (nonring)	<input type="checkbox"/>	=N- (ring)
<input type="checkbox"/>	>C= (nonring)	<input checked="" type="checkbox"/>	-CN
<input type="checkbox"/>	-CH	<input type="checkbox"/>	>S (ring)
<input type="checkbox"/>	-C- (nonring)		
<input type="checkbox"/>	>CH2 (ring)		
<input type="checkbox"/>	>CH- (ring)		
<input type="checkbox"/>	>C< (ring)		
<input type="checkbox"/>	=CH- (ring)		
<input type="checkbox"/>	>C= (ring)		
<input type="checkbox"/>	-F		
<input type="checkbox"/>	-Cl		
<input type="checkbox"/>	-Br		
<input type="checkbox"/>	-OH (alcohols)		
<input type="checkbox"/>	-O- (nonring)		
<input type="checkbox"/>	>C=O (nonring)		

Done Clear Help

Temp. Corr. Property Prediction

File Point Properties Calculate Table or Graph Help

Temperature Correlated Properties

Compound Name: ETHANOL - C2H6O

Property	Recalc	Method	Value	Prop Units	Mass Basis	Temp.	Tmin	Tmax	T Units	Tab Gph	Meth Desc
Vapor Pressure	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB	7.89567	pascal		298,15	159,1	516,3	K	<input type="checkbox"/>	Vp
Heat of Vaporization	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB		J/kmol	<input type="checkbox"/>	298,15	300,0	516,3	K	<input type="checkbox"/>	Hv
Liquid Density	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB	17,0899	kmol/m ³	<input type="checkbox"/>	298,15	159,1	516,3	K	<input type="checkbox"/>	Ld
Gas D@1,2E00 Pa	<input checked="" type="checkbox"/>	<input type="checkbox"/> Ideal	4,84078E-07	kmol/m ³	<input type="checkbox"/>	298,15			K	<input type="checkbox"/>	Gd
Surface Tension	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB	2,3386E-02	N/m		298,15	273,2	516,3	K	<input type="checkbox"/>	St
Heat of Formation	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB	-2,34881E08	J/kmol	<input type="checkbox"/>	298,15	298,0	1000,0	K	<input type="checkbox"/>	Hf
Free Energy of Formation	<input checked="" type="checkbox"/>	<input type="checkbox"/> SystemDB	-1,68512E08	J/kmol	<input type="checkbox"/>	298,15	298,0	1000,0	K	<input type="checkbox"/>	Gf
Liquid Heat Capacity	<input checked="" type="checkbox"/>	<input type="checkbox"/> Bondi-Rowlinson		J/(kmol K)	<input type="checkbox"/>	298,15	273,0	516,3	K	<input type="checkbox"/>	LCp
Gas Heat Capacity	<input checked="" type="checkbox"/>	<input type="checkbox"/> Harrison-Seaton		J/(kmol K)	<input type="checkbox"/>	298,15	300,0	1500,0	K	<input type="checkbox"/>	GCp
Solid Heat Capacity	<input checked="" type="checkbox"/>	<input type="checkbox"/> User Enter		J/(kmol K)	<input type="checkbox"/>	298,15			K	<input type="checkbox"/>	SCp
Liquid Viscosity	<input checked="" type="checkbox"/>	<input type="checkbox"/> Gambill		Pa s	<input type="checkbox"/>	298,15		413,0	K	<input type="checkbox"/>	Lv
Gas Viscosity	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> Reichenberg	6,10851E-06	Pa s	<input type="checkbox"/>	298,15			K	<input type="checkbox"/>	Gv
Liquid Therm Cond	<input checked="" type="checkbox"/>	<input type="checkbox"/> Baroncini, et al.	1,58094E-01	J/(s m K)	<input type="checkbox"/>	298,15		516,3	K	<input type="checkbox"/>	Lt
Gas Therm Cond	<input checked="" type="checkbox"/>	<input type="checkbox"/> Eucken		J/(s m K)	<input type="checkbox"/>	298,15	273,0		K	<input type="checkbox"/>	Gt

Point Property Prediction							
File Temp. Corr. Props Calculate Help							
PREDICT Chemical Physical Properties							
Compound Name: ETHANOL - C2H6O							
Property	Recalc	Method	Value	Get from DB	Units	Method	Descrip
Molecular Weight	<input checked="" type="radio"/> <input checked="" type="checkbox"/>	SystemDB	46,0684				MW
Melting Point Temperature	<input checked="" type="radio"/>	SystemDB	159,05		K		Tm
Normal Boiling Point	<input checked="" type="radio"/> <input checked="" type="checkbox"/>	SystemDB	351,44		K		Tb
Critical Temperature	<input checked="" type="radio"/> <input checked="" type="checkbox"/>	SystemDB	516,25		K		Tc
Critical Pressure	<input checked="" type="radio"/>	SystemDB	6,384E06		pascal		Pc
Critical Volume	<input checked="" type="radio"/>	SystemDB	1,669E-01		m ³ /kmol		Vc
Critical Compressibility Zc	<input checked="" type="radio"/>	SystemDB	2,48E-01				Zc
Liquid Density (Tb)	<input checked="" type="radio"/>	SystemDB	17,083		kmol/m ³		DI-Tb
Heat of Vaporization (298K)	<input checked="" type="radio"/>	Pitzer	4,32649E07		J/kmol		Hv298
Heat of Vaporization (Tb)	<input checked="" type="radio"/>	SystemDB	3,94E07		J/kmol		Hv-Tb
IG Heat of Formation (298K)	<input checked="" type="radio"/>	SystemDB	-2,3481E08		J/kmol		Hf
IG Std. Entropy (298K)	<input checked="" type="radio"/>	SystemDB	2,82590E05		J/(kmol K)		S
IG Entropy of Form (298K)	<input checked="" type="radio"/>	SystemDB	-2,23143E05		J/(kmol K)		Sf
IG Free Energy Form (298K)	<input checked="" type="radio"/>	SystemDB	-1,6828E08		J/kmol		Gf
Acentric Factor	<input checked="" type="radio"/> <input checked="" type="checkbox"/>	SystemDB	6,37E-01				Af
Polarity Factor							x
Riedel Factor	<input checked="" type="radio"/>	Riedel - Omega	8,9444				Rf