butane !short name

106-97-8 !CAS number

n-butane !full name

CH3-2(CH2)-CH3 !chemical formula {C4H10}

R-600 !synonym

58.1222 !molecular weight [g/mol]

134.895 !triple point temperature [K]

272.660 !normal boiling point [K]

425.125 !critical temperature [K]

3796.0 !critical pressure [kPa]

3.922769613 !critical density [mol/L]

0.201 !acentric factor

0.05 !dipole moment [Debye]

IIR !default reference state

8.0 !version number

1011 !UN Number

n-alkane !family

2877.40 !heating value (gross or superior) [kJ/mol]

! compiled by M. McLinden, NIST Physical and Chemical Properties Division, Boulder, Colorado

! 02-01-96 MM, original version

! 03-18-96 MM, add transport correlations compiled by S.A. Klein

! 06-17-96 MM, add thermal conductivity coefficients fitted by S.A. Klein

! 07-08-96 MM, replace temporary Cp0 with function of Younglove and Ely

! 10-03-96 MM, add surface tension fit

! 10-17-96 MM, add thermal conductivity model of Younglove and Ely

! 10-18-96 MM, missing constant in dilute-gas viscosity model

! 02-20-97 MM, add default reference state

! 02-21-97 MM, put viscosity model into revised VS2 format

! 02-26-97 MM, add version number and pointer to visc critical enhancement (both future use)

! 03-06-97 MM, modify ECS-transport to new format

! 03-25-97 MM, set Psi,Chi coeff in ECS-transport to 1,0 pending refit of data

! 08-21-97 MM, purge exponentials from values read by GUI (e.g. model limits)

! 10-24-97 MM, read in f\_int term in Eucken correlation in ECS method for t.c.

! change reference fluid EOS for ECS-transport from BWR to FEQ

! 03-24-98 EWL, set max density to triple-point density (until melting line implemented)

! 11-13-98 EWL, update format to version 6.1

! 11-18-98 EWL, add equation of state of Polt et al. (1992)

! 10-14-99 EWL, update L-J parameters

! 11-01-99 EWL, add Span 12 term short equation of state

! 11-10-99 EWL, add extra digits to melting equation to get ptp at ttp

! 11-22-99 EWL, change ECS reference fluid to nitrogen

! 01-21-00 EWL, change max density of transport eqs. to match eos

! 03-20-00 EWL, change max density to the density at p=2\*pmax along melting line

! 07-17-00 EWL, add Vogel viscosity equation

! 03-30-01 MLH, added Perkins et al. thermal conductivity equation (2001)

! 06-01-01 EWL, add Miyamoto and Watanabe equation

! 07-07-04 AHH, update dipole moment

! 08-05-04 EWL, add Harvey and Lemmon dielectric correlation

! 09-02-04 EWL, add Buecker and Wagner equation

! 10-13-04 MLH, add family

! 08-08-05 EWL, Ptrp in melting line equation changed slightly to match EOS at Ttrp

! 12-02-06 MLH, update LJ in ECS

! 03-05-07 MLH, added VS4 model

! 09-13-10 EWL, replace ancillary equations

! 10-21-10 EWL, increase upper pressure limit to 200 MPa based on data of Miyamoto (2008)

! 10-21-10 MLH, revised upper limit of pressure on vis. and therm. cond. to 200 MPa

#EOS !equation of state specification

FEQ Helmholtz equation of state for butane of Buecker and Wagner (2006).

?LITERATURE REFERENCE \

?Buecker, D. and Wagner, W.,

? "Reference Equations of State for the Thermodynamic Properties of Fluid

? Phase n-Butane and Isobutane,"

? J. Phys. Chem. Ref. Data, 35(2):929-1019, 2006.

?\

?The uncertainties in density are 0.02% at temperatures below 340 K and

?pressures below 12 MPa (both liquid and vapor states), 0.1% at temperatures

?below 270 K and pressures above 12 MPa, 0.2% between 340 and 515 K at

?pressures less than 0.6 MPa, and 0.4% elsewhere. Above the upper pressure

?limit of 69 MPa as given in the original formulation, new data up to 200 MPa

?show that the uncertainty in density is 0.3%. In the critical region,

?deviations in pressure are 0.5%. At temperatures above 500 K, the

?uncertainties in density increase up to 1%. Uncertainties in heat capacities

?are typically 1%, rising to 5% in the critical region and at pressures above

?30 MPa. Uncertainties in the speed of sound are typically 0.5%, rising to 1%

?at temperatures below 200 K and to 4% in a large area around the critical

?point.

?\

!end of info section

134.895 !lower temperature limit [K]

575.0 !upper temperature limit [K]

200000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

CPP !pointer to Cp0 model

58.1222 !molecular weight [g/mol]

134.895 !triple point temperature [K]

0.000653 !pressure at triple point [kPa]

12.645 !density at triple point [mol/L]

272.660 !normal boiling point temperature [K]

0.201 !acentric factor

425.125 3796.0 3.922769613 !Tc [K], pc [kPa], rhoc [mol/L]

425.125 3.922769613 !reducing parameters [K, mol/L]

8.314472 !gas constant [J/mol-K]

23 4 2 12 0 0 !# terms, # coeff/term for: "normal" terms, critical, spare

.25536998241635D+01 0.5 1. 0 !a(i),t(i),d(i),l(i)

-.44585951806696D+01 1.0 1. 0

.82425886369063D+00 1.5 1. 0

.11215007011442D+00 0.0 2. 0

-.35910933680333D-01 0.5 3. 0

.16790508518103D-01 0.5 4. 0

.32734072508724D-01 0.75 4. 0

.95571232982005D+00 2.0 1. 1

-.10003385753419D+01 2.5 1. 1

.85581548803855D-01 2.5 2. 1

-.25147918369616D-01 1.5 7. 1

-.15202958578918D-02 1.0 8. 1

.47060682326420D-02 1.5 8. 1

-.97845414174006D-01 4.0 1. 2

-.48317904158760D-01 7.0 2. 2

.17841271865468D+00 3.0 3. 2

.18173836739334D-01 7.0 3. 2

-.11399068074953D+00 3.0 4. 2

.19329896666669D-01 1.0 5. 2

.11575877401010D-02 6.0 5. 2

.15253808698116D-03 0.0 10. 2

-.43688558458471D-01 6.0 2. 3

-.82403190629989D-02 13.0 6. 3

-.28390056949441D-01 2.0 1. 2 2 -10. -150. 1.16 .85 0. 0. 0.

.14904666224681D-02 0.0 2. 2 2 -10. -200. 1.13 1. 0. 0. 0.

#AUX !auxiliary model specification

CPP ideal gas heat capacity function

?LITERATURE REFERENCE \

?see Buecker and Wagner EOS for reference

?\

!end of info section

134.895 !lower temperature limit [K]

575.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1.0 8.314472 !reducing parameters for T, Cp0

1 4 0 0 0 0 0 !Nterms: polynomial, exponential, cosh, sinh

4.24680487 0.00000

5.54913289 329.40404

11.4648996 1420.17366

7.59987584 2113.08938

9.66033239 4240.85730

@EOS !equation of state specification

FEK Helmholtz equation of state for butane of Kunz and Wagner (2004).

?LITERATURE REFERENCE \

?Kunz, O., Klimeck, R., Wagner, W., Jaeschke, M.

? "The GERG-2004 Wide-Range Equation of State for Natural Gases

? and Other Mixtures," GERG Technical Monograph 15,

? Fortschritt-Berichte VDI, VDI-Verlag, Düsseldorf, 2007.

?\

!end of info section

134.895 !lower temperature limit [K]

575.0 !upper temperature limit [K]

69000.0 !upper pressure limit [kPa]

13.2 !maximum density [mol/L]

PHK !pointer to Cp0 model

58.1222 !molecular weight [g/mol]

134.895 !triple point temperature [K]

1. !pressure at triple point [kPa]

1. !density at triple point [mol/L]

272.62 !normal boiling point temperature [K]

0.2038 !acentric factor

425.125 3830.3 3.920016792 !Tc [K], pc [kPa], rhoc [mol/L]

425.125 3.920016792 !reducing parameters [K, mol/L]

8.314472 !gas constant [J/mol-K]

12 4 0 0 0 0 !# terms, # coeff/term for: "normal" terms, critical, spare

0.10626277411455d1 0.250 1. 0

-0.28620951828350d1 1.125 1. 0

0.88738233403777 1.500 1. 0

-0.12570581155345 1.375 2. 0

0.10286308708106 0.250 3. 0

0.25358040602654d-3 0.875 7. 0

0.32325200233982 0.625 2. 1

-0.37950761057432d-1 1.750 5. 1

-0.32534802014452 3.625 1. 2

-0.79050969051011d-1 3.625 4. 2

-0.20636720547775d-1 14.5 3. 3

0.57053809334750d-2 12.0 4. 3

#AUX !auxiliary model specification

PHK Helmholtz form for the ideal-gas state for butane of Kunz and Wagner (2004).

?LITERATURE REFERENCE \

?Kunz, O., Klimeck, R., Wagner, W., Jaeschke, M.

? "The GERG-2004 Wide-Range Equation of State for Natural Gases

? and Other Mixtures," GERG Technical Monograph 15,

? Fortschritt-Berichte VDI, VDI-Verlag, Düsseldorf, 2007.

?\

!end of info section

0. !lower temperature limit [K]

1000.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1 2 0 2 2 0 0 0 !Nterms: ai\*log(tau\*\*ti); ai\*tau\*\*ti; ai\*log(1-exp(bi\*tau)); cosh; sinh

3.33944 1. !ai, ti for [ai\*log(tau\*\*ti)] terms

20.884143364 0. !aj, ti for [ai\*tau\*\*ti] terms

-91.638478026 1.

-6.89406 0.43195766 !aj, ti for cosh and sinh terms

-14.7824 2.124516319

9.44893 1.101487798

24.4618 4.502440459

#AUX !auxiliary model specification

PH0 Helmholtz form for the ideal-gas state

?LITERATURE REFERENCE \

?\

!end of info section

134.895 !lower temperature limit [K]

575.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1 2 4 0 0 0 0 0 !Nterms: ai\*log(tau\*\*ti); ai\*tau\*\*ti; ai\*log(1-exp(bi\*tau))

3.24680487 1. !ai, ti for [ai\*log(tau\*\*ti)] terms

12.54882924 0. !aj, ti for [ai\*tau\*\*ti] terms

-5.46976878 1.

5.54913289 -0.7748404445 !aj, ti for [ai\*log(1-exp(ti\*tau)] terms

11.4648996 -3.3406025522

7.59987584 -4.9705130961

9.66033239 -9.9755537783

@EOS !equation of state specification

FE1 Helmholtz equation of state for butane of Miyamoto and Watanabe (2001).

?LITERATURE REFERENCE \

?Miyamoto, H. and Watanabe, K.

? "A Thermodynamic Property Model for Fluid-Phase n-Butane,"

? Int. J. Thermophys., 22(2):459-475, 2001.

?\

?The uncertainties of the equation of state are approximately 0.2%

?in density, 1% in heat capacity, 1% in the speed of sound, and

?0.2% in vapor pressure, except in the critical region.

?\

!end of info section

134.87 !lower temperature limit [K]

589.0 !upper temperature limit [K]

69000 !upper pressure limit [kPa]

13.15 !maximum density [mol/L]

CP1 !pointer to Cp0 model

58.1222 !molecular weight [g/mol]

134.87 !triple point temperature [K]

0.000688 !pressure at triple point [kPa]

12.652 !density at triple point [mol/L]

272.6 !normal boiling point temperature [K]

0.2 !acentric factor

425.125 3796.0 3.92001679 !Tc [K], pc [kPa], rhoc [mol/L]

425.125 3.92001679 !reducing parameters [K, mol/L]

8.314472 !gas constant [J/mol-K]

19 4 0 0 0 0 !# terms, # coeff/term for: "normal" terms, critical, spare

2.952054E-01 -0.25 1.0 0 !a(i),t(i),d(i),l(i)

-1.326360E+00 1.50 1.0 0

-2.031317E-03 -0.75 2.0 0

2.240301E-01 0.00 2.0 0

-3.635425E-02 1.25 3.0 0

1.905841E-03 1.50 5.0 0

7.409154E-05 0.50 8.0 0

-1.401175E-06 2.50 8.0 0

-2.492172E+00 1.50 3.0 1

2.386920E+00 1.75 3.0 1

1.424009E-03 -0.25 8.0 1

-9.393388E-03 3.00 5.0 1

2.616590E-03 3.00 6.0 1

-1.977323E-01 4.00 1.0 2

-3.809534E-02 2.00 5.0 2

1.523948E-03 -1.00 7.0 2

-2.391345E-02 2.00 2.0 3

-9.535229E-03 19.00 3.0 3

3.928384E-05 5.00 15.0 3

#AUX !auxiliary model specification

CP1 ideal gas heat capacity function

?LITERATURE REFERENCE \

?Miyamoto, H. and Watanabe, K.

? "A Thermodynamic Property Model for Fluid-Phase n-Butane,"

? Int. J. Thermophys., 22(2):459-475, 2001.

?\

!end of info section

134.87 !lower temperature limit [K]

589.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1.0 8.3144720 !reducing parameters for T, Cp0

1 4 0 0 0 0 0 !Nterms: polynomial, exponential, cosh, sinh

4.240207 0.00000

5.513671 327.55988

7.388450 1319.06935

10.250630 4138.63184

11.061010 1864.36783

@EOS !equation of state specification

BWR MBWR equation of state for butane of Younglove and Ely (1987).

?LITERATURE REFERENCE \

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

?The uncertainties in density are 0.05% in the liquid, 0.4% in the vapor

?and 0.06% in the supercritical and critical regions. The uncertainty is

?2% for heat capacities, 1% for the speed of sound in the vapor, and 2%

?for the speed of sound in the liquid.

?\

?N.B. all temperatures on IPTS-68

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

70000.0 !upper pressure limit [kPa]

13.20 !maximum density [mol/L]

CP2 !pointer to Cp0 model

58.1222 !molecular weight [g/mol]

134.86 !triple point temperature [K]

6.736d-4 !pressure at triple point [kPa]

12.650 !density at triple point [mol/L]

272.613 !normal boiling point temperature [K]

0.199586 !acentric factor

425.16 3796. 3.920 !Tc [K], pc [kPa], rhoc [mol/L]

425.16 3.920 !reducing parameters [K, mol/L]

3.920 !gamma

0.0831434 !gas constant [L-bar/mol-K]

32 1 !Nterm, Ncoeff per term

0.153740104603d-01 -0.160980034611d+00 -0.979782459010d+01

0.499660674504d+03 -0.102115607687d+07 0.236032147756d-02

-0.137475757093d+01 -0.907038733865d+03 0.385421748213d+06

-0.349453710700d-04 0.157361122714d+00 0.102301474068d+03

0.182335737331d-01 -0.404114307787d+01 0.187979855783d+01

0.362088795040d+00 -0.738762248266d-02 -0.218618590563d+01

0.118802729027d+00 0.706854198713d+06 -0.219469885796d+09

-0.182454361268d+05 0.206790377277d+10 0.111757550145d+03

0.558779925986d+05 -0.159579054026d+02 -0.148034214622d+07

-0.245206328201d+00 0.218305259309d+03 -0.923990627338d-04

-0.205267776639d+01 0.387639044820d+02

#AUX !auxiliary model specification

CP2 ideal gas heat capacity function of Younglove and Ely

?LITERATURE REFERENCE \

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1.0 8.31434 !reducing parameters for T, Cp0

7 1 0 0 0 0 0 !Nterms: polynomial, exponential, cosh, sinh

3.8802310194d+5 -3.00d0

-1.5444296890d+5 -2.00d0

2.8455082239d+3 -1.00d0

-1.3491511376d+1 0.00d0

6.6142595353d-2 1.00d0

-2.4307965028d-5 2.00d0

1.5044248429d-10 3.00d0

-8.3933423467d+0 3000.d0

@EOS !equation of state specification

FES short Helmholtz equation of state for butane of Span and Wagner (2003).

?LITERATURE REFERENCE \

?Span, R. and Wagner, W.

? "Equations of State for Technical Applications. II. Results for Nonpolar Fluids,"

? Int. J. Thermophys., 24(1):41-109, 2003.

?\

?The uncertainties of the equation of state are approximately 0.2% (to

?0.5% at high pressures) in density, 1% (in the vapor phase) to 2% in

?heat capacity, 1% (in the vapor phase) to 2% in the speed of sound, and

?0.2% in vapor pressure, except in the critical region.

?\

!end of info section

134.86 !lower temperature limit [K]

600.0 !upper temperature limit [K]

100000.0 !upper pressure limit [kPa]

13.20 !maximum density [mol/L]

CPS !pointer to Cp0 model

58.123 !molecular weight [g/mol]

134.86 !triple point temperature [K]

0.00064578 !pressure at triple point [kPa]

12.671 !density at triple point [mol/L]

272.62 !normal boiling point temperature [K]

0.2 !acentric factor

425.125 3796.0 3.9199628 !Tc [K], pc [kPa], rhoc [mol/L]

425.125 3.9199628 !reducing parameters [K, mol/L]

8.31451 !gas constant [J/mol-K]

12 4 0 0 0 0 !# terms, # coeff/term for: "normal" terms, critical, spare

0.106262770000E+01 0.25 1.0 0 !a(i),t(i),d(i),l(i)

-0.286209520000E+01 1.125 1.0 0

0.887382330000E+00 1.5 1.0 0

-0.125705810000E+00 1.375 2.0 0

0.102863090000E+00 0.25 3.0 0

0.253580410000E-03 0.875 7.0 0

0.323252000000E+00 0.625 2.0 1

-0.379507610000E-01 1.75 5.0 1

-0.325348020000E+00 3.625 1.0 2

-0.790509690000E-01 3.625 4.0 2

-0.206367210000E-01 14.5 3.0 3

0.570538090000E-02 12.0 4.0 3

#AUX !auxiliary model specification

CPS ideal gas heat capacity function

?LITERATURE REFERENCE \

?Jaeschke, M. and Schley, P.

? "Ideal-Gas Thermodynamic Properties for Natural-Gas Applications,"

? Int. J. Thermophys., 16(6):1381-1392, 1995.

?\

!end of info section

134.86 !lower temperature limit [K]

600.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1.0 8.31451 !reducing parameters for T, Cp0

1 0 2 2 0 0 0 !Nterms: polynomial, exponential, cosh, sinh

0.4339440E+01 0.0

0.2324827E+06 -2.0 0.1836360E+03 -1.0 -2.0

0.1205864E+08 -2.0 0.9031850E+03 -1.0 -2.0

0.2071931E+07 -2.0 0.4682700E+03 -1.0 -2.0

0.8962262E+08 -2.0 0.1914100E+04 -1.0 -2.0

@EOS !equation of state specification

FE3 Helmholtz equation of state for butane of Polt et al. (1992).

?LITERATURE REFERENCE \

?Polt, A., Platzer, B., and Maurer, G.,

? "Parameter der thermischen Zustandsgleichung von Bender fuer 14

? mehratomige reine Stoffe,"

? Chem. Tech. (Leipzig), 44(6):216-224, 1992.

?\

!end of info section

140.0 !lower temperature limit [K]

589.0 !upper temperature limit [K]

30000.0 !upper pressure limit [kPa]

12.81 !maximum density [mol/L]

CP3 !pointer to Cp0 model

58.124 !molecular weight [g/mol]

140.0 !triple point temperature [K]

0.00161 !pressure at triple point [kPa]

12.573 !density at triple point [mol/L]

272.62 !normal boiling point temperature [K]

0.1984 !acentric factor

425.14 3783.85 3.9192072 !Tc [K], pc [kPa], rhoc [mol/L]

425.14 3.9192072 !reducing parameters [K, mol/L]

8.3143 !gas constant [J/mol-K]

22 5 0 0 0 0 !# terms, # coeff/term for: "normal" terms, critical, spare

-0.504188295325d+0 3.0 0.0 0 0.0 !a(i),t(i),d(i),l(i)

0.541067401063d+0 4.0 0.0 0 0.0

-0.760421383062d-1 5.0 0.0 0 0.0

0.846035653528d+0 0.0 1.0 0 0.0

-0.191317317203d+1 1.0 1.0 0 0.0

0.521441860186d+0 2.0 1.0 0 0.0

-0.783511318207d+0 3.0 1.0 0 0.0

0.689697797175d-1 4.0 1.0 0 0.0

0.947825461055d-1 0.0 2.0 0 0.0

-0.141401831669d+0 1.0 2.0 0 0.0

0.382675021672d+0 2.0 2.0 0 0.0

-0.423893176684d-1 0.0 3.0 0 0.0

0.677591792029d-1 1.0 3.0 0 0.0

0.567943363340d-1 0.0 4.0 0 0.0

-0.131517698401d+0 1.0 4.0 0 0.0

0.221136942526d-1 1.0 5.0 0 0.0

0.504188295325d+0 3.0 0.0 2 1.08974964

-0.541067401063d+0 4.0 0.0 2 1.08974964

0.760421383062d-1 5.0 0.0 2 1.08974964

-0.619109535460d-1 3.0 2.0 2 1.08974964

0.423035373804d+0 4.0 2.0 2 1.08974964

-0.390505508895d+0 5.0 2.0 2 1.08974964

#AUX !auxiliary model specification

CP3 ideal gas heat capacity function

?LITERATURE REFERENCE \

?Polt, A., Platzer, B., and Maurer, G.,

? "Parameter der thermischen Zustandsgleichung von Bender fuer 14

? mehratomige reine Stoffe,"

? Chem. Tech. (Leipzig), 44(6):216-224, 1992.

?\

!end of info section

140.0 !lower temperature limit [K]

589.0 !upper temperature limit [K]

0.0 !upper pressure limit [kPa]

0.0 !maximum density [mol/L]

1.0 58.124 !reducing parameters for T, Cp0

5 0 0 0 0 0 0 !Nterms: polynomial, exponential, cosh, sinh

0.801601d+00 0.00

0.655936d-03 1.00

0.122770d-04 2.00

-0.165626d-07 3.00

0.677360d-11 4.00

#TCX !thermal conductivity model specification

TC1 pure fluid thermal conductivity model of Perkins et al. (2002).

?LITERATURE REFERENCE \

?Perkins, R.A, Ramires, M.L.V., Nieto de Castro, C.A. and Cusco, L.,

? "Measurement and Correlation of the Thermal Conductivity of Butane

? from 135 K to 600 K at Pressures to 70 MPa,"

? J. Chem. Eng. Data, 47(5):1263-1271, 2002.

?\

?Uncertainty in thermal conductivity is 3%, except in the critical region

? and dilute gas which have an uncertainty of 5%.

?\

!end of info section

134.86 !lower temperature limit [K]

600.0 !upper temperature limit [K]

200000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

3 0 !# terms for dilute gas function: numerator, denominator

425.16 1.0 !reducing parameters for T, tcx

1.62676d-3 0.00d0 !coeff, power in T

9.75703d-4 1.00d0

2.89887d-2 2.00d0

10 0 !# terms for background gas function: numerator, denominator

425.16 3.92 1.0 !reducing par for T, rho, tcx

-3.04337d-2 0.0 1.0 0.0 !coeff, powers of T, rho, spare for future use

4.18357d-2 1.00d0 1.00d0 0.00d0

1.65820d-1 0.00d0 2.00d0 0.00d0

-1.47163d-1 1.00d0 2.00d0 0.00d0

-1.48144d-1 0.00d0 3.00d0 0.00d0

1.33542d-1 1.00d0 3.00d0 0.00d0

5.25500d-2 0.00d0 4.00d0 0.00d0

-4.85489d-2 1.00d0 4.00d0 0.00d0

-6.29367d-3 0.00d0 5.00d0 0.00d0

6.44307d-3 1.00d0 5.00d0 0.00d0

TK3 !pointer to critical enhancement auxiliary function

#AUX !thermal conductivity critical enhancement model

TK3 thermal conductivity critical enhancement of Perkins et al. (2002).

?LITERATURE REFERENCE \

?Perkins, R.A., Ramires, M.L.V., Castro de Nieto, C.A. and Cusco, L.,

? "Measurement and Correlation of the Thermal Conductivity of Butane

? from 135 K to 600 K at Pressures to 70 MPa,"

? J. Chem. Eng. Data, 47(5):1263-1271, 2002.

?\

!end of info section

134.86 !lower temperature limit [K]

600.0 !upper temperature limit [K]

200000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

9 0 0 0 !# terms: terms, spare, spare, spare

1.0 1.0 1.0 !reducing par for T, rho, tcx (mW/m-K)

0.630d0 !gnu (universal exponent)

1.239d0 !gamma (universal exponent)

1.03d0 !R0 (universal amplitude)

0.063d0 !z (universal exponent--not used for t.c., only viscosity)

1.00d0 !c (constant in viscosity eqn = 1/[2 - (alpha + gamma)/(2\*nu)], but often set to 1)

0.194d-9 !xi0 (amplitude) [m]

0.0496 !gam0 (amplitude) [-]

0.875350d-9 !qd\_inverse (modified effective cutoff parameter) [m]

637.68 !tref (reference temperature) [K]

@TCX !thermal conductivity model specification

TC2 pure fluid thermal conductivity model of Younglove and Ely (1987).

?LITERATURE REFERENCE \

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

?The uncertainty in thermal conductivity is 2%, except in the critical region

?which is 10%.

?\

?N.B. all temperatures on IPTS-68

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

70000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

CI2 !pointer to collision integral model

0.503103 !Lennard-Jones coefficient sigma [nm]

440.0 !Lennard-Jones coefficient epsilon/kappa [K]

2.0352526600d-01 !const in Eq 19 = 5/16\*(k\*MW/1000/pi/Na)\*\*0.5\*1.0d12

0.1530992335d+01 !dilute gas terms (Eq 27): Gt(1)

-0.2114511021d+00 ! Gt(2)

0.4024170074d-02 !residual terms (Eqs 26, 28-30): Et(1)

0.1561435847d+01

-0.6004381127d+03

-0.7547260841d-03

-0.2069676662d-01

0.9382534978d+02

-0.1711371457d+00

0.3647724935d+02 !Et(8)

TK2 !pointer to critical enhancement model (follows immediately)

0.000769608d0 !critical enhancement terms (Eqs D1-D4): X1

13.2533d0

0.485554d0

1.01021d0 !X4

9.10218d-10 !Z

1.38054d-23 !Boltzmann's constant, k

0.1630521851d+01 !coeff for initial density dependence of viscosity (eq 21); Fv(1)

0.0 !Fv(2)

1.40 !Fv(3)

425.16 !Fv(4)

-0.2724386845d+02 !coefficients for residual viscosity, eqs (22 - 25)

0.8012766611d+03 !Ev(2) (the viscosity is also used in conductivity correlation)

0.2503978646d+02 !Ev(3)

-0.1309704275d+05 !Ev(4)

-0.8313305258d-01 !Ev(5)

0.6636975027d+02 !Ev(6)

0.9849317662d+04 !Ev(7)

#ETA !viscosity model specification

VS1 pure fluid viscosity model of Vogel et al. (1999).

?LITERATURE REFERENCE \

?Vogel, E., Kuechenmeister, C., and Bich, E.,

? "Viscosity for n-Butane in the Fluid Region,"

? High Temp. - High Pressures, 31(2):173-186, 1999.

?\

?The uncertainty in viscosity varies from 0.4% in the dilute gas between

?room temperature and 600 K, to 3.0% over the rest of the fluid surface.

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

200000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

1 !number of terms associated with dilute-gas function

CI1 !pointer to reduced effective collision cross-section model

0.57335 !Lennard-Jones coefficient sigma [nm]

280.51 !Lennard-Jones coefficient epsilon/kappa [K]

1.0 1.0 !reducing parameters for T, eta

0.1628213 0.50d0 !Chapman-Enskog term

9 !number of terms for initial density dependence

280.51 0.1135034 !reducing parameters for T (= eps/k), etaB2 (= 0.6022137\*sigma\*\*3)

-19.572881d0 0.0 !coeff, power in T\* = T/(eps/k)

219.73999d0 -0.25

-1015.3226d0 -0.5

2471.01251d0 -0.75

-3375.1717d0 -1.0

2491.6597d0 -1.25

-787.26086d0 -1.5

14.085455d0 -2.5

-0.34664158d0 -5.5

2 13 1 2 0 0 !# resid terms: close-packed density; simple poly; numerator of rational poly; denominator of rat. poly; numerator of exponential; denominator of exponential

425.125 3.92 1.0 !reducing parameters for T, rho, eta

2.30873963359 0.0 0.00 0.00 0

2.03404037254 0.5 0.00 0.00 0

-54.7737770846 0.0 2.00 0.00 0

58.0898623034 -1.0 2.00 0.00 0

0 -2.0 2.00 0.00 0

35.2658446259 0.0 3.00 0.00 0

-39.6682203832 -1.0 3.00 0.00 0

0 -2.0 3.00 0.00 0

-1.83729542151 0.0 4.00 0.00 0

0 -1.0 4.00 0.00 0

0 -2.0 4.00 0.00 0

-0.833262985358 0.0 5.00 0.00 0

1.93837020663 -1.0 5.00 0.00 0

0 -2.0 5.00 0.00 0

-188.075903903 0.0 1.00 -1.00 0

188.075903903 0.0 1.00 0.00 0

1. 0.0 0.00 1.00 0

-1. 0.0 1.00 0.00 0

NUL !pointer to critical enhancement auxiliary function (none used)

#AUX !collision integral specification

CI1 collision integral model of Vogel et al. (1999).

?LITERATURE REFERENCE \

?Vogel, E., Kuechenmeister, C., and Bich, E.,

? "Viscosity for n-Butane in the Fluid Region,"

? High Temp. - High Pressures, 31(2):173-186, 1999.

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

3 !number of terms

0.17067154 0 !coeff, power of Tstar

-0.48879666 1

0.039038856 2

@ETA !viscosity model specification

VS2 pure fluid viscosity model of Younglove and Ely (1987).

?LITERATURE REFERENCE \

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

?The uncertainty in viscosity is 2%, except in the critical region which is 5%.

?\

?N.B. all temperatures on IPTS-68

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

70000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

CI2 !pointer to collision integral model

0.503103 !Lennard-Jones coefficient sigma [nm]

440.0 !Lennard-Jones coefficient epsilon/kappa [K]

2.0352457000d-01 !const in Eq 19 = 5/16\*(k\*MW/1000/pi/Na)\*\*0.5\*1.0d12

0.5 !exponent in Eq 19 for T

0.1630521851d+01 !coeff for initial density dependence of viscosity (eq 21); Fv(1)

0.0 !Fv(2)

1.40 !Fv(3)

425.16 !Fv(4)

-0.2724386845d+02 !coefficients for residual viscosity, eqs (22 - 25)

0.8012766611d+03 !Ev(2)

0.2503978646d+02 !Ev(3)

-0.1309704275d+05 !Ev(4)

-0.8313305258d-01 !Ev(5)

0.6636975027d+02 !Ev(6)

0.9849317662d+04 !Ev(7)

3.920 !Ev(8)

NUL !pointer to critical enhancement auxiliary function (none used)

#AUX !collision integral specification

CI2 collision integral model of Younglove and Ely (1987).

?LITERATURE REFERENCE \

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

?N.B. all temperatures on IPTS-68

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

9 !number of terms

-3.0328138281 !Omega (eq 20): coeffs of {(e/kT)\*\*((4-n)/3)}

16.918880086 !N.B. there is misprint in Younglove and Ely, the exponent

-37.189364917 ! is ((4-n)/3) not ((n+2)/3)

41.288861858

-24.61592114

8.948843096

-1.8739245042

0.209661014 !N.B. wrong sign in Younglove and Ely, Table 2

-0.009657044

@ETA !viscosity model specification

VS4 pure fluid generalized friction theory viscosity model of Quinones-Cisneros and Deiters (2006).

?LITERATURE REFERENCE \

? Quinones-Cisneros, S.E. and Deiters, U.K.

? "Generalization of the Friction Theory for Viscosity Modeling,"

? J. Phys. Chem. B, 110:12820-12834, 2006.

?

!end of info section

134.895 !lower temperature limit [K]

500.0 !upper temperature limit [K]

68000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

4 0 0 0 0 0 !number of terms associated with dilute-gas function

NUL !pointer to reduced effective collision cross-section model;not used

0.503103 !Lennard-Jones coefficient sigma [nm] (not used)

440.0 !Lennard-Jones coefficient epsilon/kappa [K] (not used)

425.125d0 1.0d0 !reducing parameters for T, eta

0.0d0 0.5d0 !Chapman-Enskog term; not used here

18.3983d0 0.0d0 !empirical terms for eta0

-57.1255d0 0.25d0

49.3197d0 0.5d0

0 !number of terms for initial density dependence; not yet used.

-1.34110938674421d-05 -8.56587924603951d-05 -6.45720639242339d-13 !a(0),a(1),a(2)

1.49859653515567d-04 -1.71133855507542d-04 7.37953726544736d-13 !b(0),b(1),b(2)

3.53018109777015d-07 -1.93040375218067d-05 -1.26469933968355d-14 !c(0),c(1),c(2)

-3.63389393526204d-09 -7.73717469888952d-10 0.00000000000000d+00 !A(0),A(1),A(2)

3.70980259815724d-08 2.07658634467549d-09 0.00000000000000d+00 !B(0),B(1),B(2)

-1.12495594619911d-07 7.66906137372152d-08 0.00000000000000d+00 !C(0),C(1),C(2)

0.0d0 0.0d0 0.0d0 !D(0),D(1),D(2)

NUL !pointer to critical enhancement auxiliary function (none used)

@TRN !transport model specification

ECS Extended Corresponding States model (Nitrogen reference); predictive mode.

?LITERATURE REFERENCES \

?Klein, S.A., McLinden, M.O., and Laesecke, A.,

? "An improved extended corresponding states method for estimation of

? viscosity of pure refrigerants and mixtures,"

? Int. J. Refrigeration, 20:208-217, 1997.

?\

?McLinden, M.O., Klein, S.A., and Perkins, R.A.,

? "An extended corresponding states model for the thermal conductivity

? of refrigerants and refrigerant mixtures,"

? Int. J. Refrigeration, 23:43-63, 2000.

?\

?Thermal conductivity and viscosity data used in the development of the

?extended corresponding states correlations were taken from:

?\

?Younglove, B.A. and Ely, J.F.,

? "Thermophysical properties of fluids. II. Methane, ethane, propane,

? isobutane and normal butane,"

? J. Phys. Chem. Ref. Data, 16:577-798, 1987.

?\

?the Lennard-Jones parameters are taken from:

?\

?Reid, R.C., Prausnitz, J.M., and Poling, B.E.,

? "The Properties of Gases and Liquids,"

? 4th edition, New York, McGraw-Hill Book Company, 1987.

?\

!end of info section

134.86 !lower temperature limit [K]

500.0 !upper temperature limit [K]

70000.0 !upper pressure limit [kPa]

13.86 !maximum density [mol/L]

FEQ nitrogen.fld

VS1 !model for reference fluid viscosity

TC1 !model for reference fluid thermal conductivity

1 !Lennard-Jones flag (0 or 1) (0 => use estimates)

0.57335 !Lennard-Jones coefficient sigma [nm]

280.51 !Lennard-Jones coefficient epsilon/kappa [K]

1 0 0 !number of terms in f\_int term in Eucken correlation, spare1, spare2

1.32d-3 0.0 0.0 0.0 !coeff, power of T, spare 1, spare 2

1 0 0 !number of terms in psi (visc shape factor): poly,spare1,spare2

1.0 0.0 0.0 0.0 !coeff, power of Tr, power of Dr, spare

1 0 0 !number of terms in chi (t.c. shape factor): poly,spare1,spare2

1.0 0.0 0.0 0.0 !coeff, power of Tr, power of Dr, spare

NUL !pointer to critical enhancement auxiliary function

#STN !surface tension specification

ST1 surface tension model; fit of data from Calado (1978) and Coffin (1928).

?LITERATURE REFERENCE \

?Fit of data from:

?\

?Calado, J.C.G., McLure, I.A., and Soares, V.A.M.,

? "Surface tension for octafluorocyclobutane, n-butane and their mixtures

? from 233 K to 254 K, and vapour pressure, excess Gibbs function and excess

? volume for the mixture at 233 K,"

? Fluid Phase Equilibria, 2:199-213, 1978.

?\

?Coffin, C.C. and Maass, O.,

? "The preparation and physical properties of alpha-, beta- and gamma-

? butylene and normal and isobutane,"

? J. Am. Chem. Soc., 50:1427-1437, 1928.

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

1 !number of terms in surface tension model

425.125 !critical temperature used in fit (dummy)

0.05418 1.26 !sigma0 and n

#DE !dielectric constant specification

DE3 dielectric constant model of Harvey and Lemmon (2005).

?LITERATURE REFERENCE \

?Harvey, A.H. and Lemmon, E.W.

? "Method for Estimating the Dielectric Constant of Natural Gas Mixtures,"

? Int. J. Thermophys., 26(1):31-46, 2005.

?\

!end of info section

0.0 !lower temperature limit [K]

2000.0 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

273.16 1000.0 1.0 !reducing parameters for t and d

1 2 4 0 0 0 !number of terms in dielectric constant model

0.0557549 -1. 1. 0. !coef, t exp, d exp

20.611 0. 1. 0.

0.020 1. 1. 0.

66.64 0. 2. 0.

24.44 1. 2. 0.

-7461.2 0. 3. 0.

-1983.6 1. 3. 0.

#MLT !melting line specification

ML1 melting line model of Buecker and Wagner (2005).

?LITERATURE REFERENCE \

? see EOS for reference

?\

!end of info section

134.895 !lower temperature limit [K]

575.0 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

134.895 0.00066566 !reducing temperature and pressure

2 0 0 0 0 0 !number of terms in melting line equation

-558558235.4 0. !coefficients and exponents

558558236.4 2.206

#PS !vapor pressure equation

PS5 vapor pressure equation of Lemmon (2010).

?LITERATURE REFERENCE \

?Lemmon, E.W., 2010.

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3796.0 !reducing parameters

4 0 0 0 0 0 !number of terms in equation

-0.71897D+01 1.0 !coefficients and exponents

0.26122D+01 1.5

-0.21729D+01 2.0

-0.27230D+01 4.5

#DL !saturated liquid density equation

DL1 saturated liquid density equation of Lemmon (2010).

?LITERATURE REFERENCE \

?Lemmon, E.W., 2010.

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3.922769613 !reducing parameters

4 0 0 0 0 0 !number of terms in equation

0.52341D+01 0.44 !coefficients and exponents

-0.62011D+01 0.60

0.36063D+01 0.76

0.22137D+00 5.00

#DV !saturated vapor density equation

DV3 saturated vapor density equation of Lemmon (2010).

?LITERATURE REFERENCE \

?Lemmon, E.W., 2010.

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3.922769613 !reducing parameters

5 0 0 0 0 0 !number of terms in equation

-0.27390D+01 0.391 !coefficients and exponents

-0.57347D+01 1.14

-0.16408D+02 3.0

-0.46986D+02 6.5

-0.10090D+03 14.0

@END

c 1 2 3 4 5 6 7 8

c2345678901234567890123456789012345678901234567890123456789012345678901234567890

#PS !vapor pressure equation

PS5 vapor pressure equation of Buecker and Wagner (2005).

?LITERATURE REFERENCE \

?See EOS

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3796.0 !reducing parameters

4 0 0 0 0 0 !number of terms in equation

-7.17616903 1.0 !coefficients and exponents

2.53635336 1.5

-2.07532869 2.0

-2.82241113 4.5

#DL !saturated liquid density equation

DL1 saturated liquid density equation of Buecker and Wagner (2005).

?LITERATURE REFERENCE \

?See EOS

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3.922769613 !reducing parameters

4 0 0 0 0 0 !number of terms in equation

1.97874515 0.345 !coefficients and exponents

0.856799510 1.0

-0.341871887 1.5

0.304337558 3.0

#DV !saturated vapor density equation

DV6 saturated vapor density equation of Buecker and Wagner (2005).

?LITERATURE REFERENCE \

?See EOS

?\

!end of info section

134.895 !lower temperature limit [K]

425.125 !upper temperature limit [K]

0.0 !(dummy) upper pressure limit

0.0 !(dummy) maximum density

425.125 3.922769613 !reducing parameters

4 0 0 0 0 0 !number of terms in equation

-2.07770057 1.035 !coefficients and exponents

-3.08362490 2.5

-0.485645266 9.5

-3.83167519 12.5