

butane	!short name
106-97-8	!CAS number
n-butane	!full name
CH <sub>3</sub> -2(CH <sub>2</sub> )-CH <sub>3</sub>	!chemical formula {C <sub>4</sub> H <sub>10</sub> }
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  $p=2*p_{max}$  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

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#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.

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#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

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@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

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#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

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#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

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@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

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#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

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@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

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#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

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@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

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#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

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@EOS                      !equation of state specification
FE3  Helmholtz equation of state for butane of Polt et al. (1992).
?LITERATURE REFERENCE \
?Polt, A., Platzner, 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

c23456789012345678901234567890123456789012345678901234567890123456789

0

```
#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
```