

isobutane	!short name
75-28-5	!CAS number
2-methylpropane	!full name
CH(CH ₃) ₃	!chemical formula {C ₄ H ₁₀ }
R-600a	!synonym
58.1222	!molecular weight [g/mol]
113.73	!triple point temperature [K]
261.401	!normal boiling point [K]
407.81	!critical temperature [K]
3629.0	!critical pressure [kPa]
3.879756788	!critical density [mol/L]
0.184	!acentric factor
0.132	!dipole moment [Debye]; DIPPR: from Nelson, NBS, NSRDS 10
(1967).	
IIR	!default reference state
8.0	!version number
1969	!UN Number
br-alkane	!family
2868.20	!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

! 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

! 07-19-96 MM, fix bug on L-J flag for ECS-transport coeff

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

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

! 10-24-96 MM, add thermal conductivity model of Younglove and Ely

! 10-25-96 MM, add collision integral of Younglove and Ely (needed for conductivity)

! missing Fv(1) in viscosity model

! 01-31-97 MM, change pointer for ECS reference viscosity from VS3 to VS1

! 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)

! 03-11-97 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

! 01-24-00 EWL, increase max density slightly in 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

! 03-29-01 MLH, new thermal conductivity correlation for ic4 added (Perkins, 2001)

! 05-14-01 EWL, add Miyamoto and Watanabe equation

! 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, updated LJ for ECS

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#EOS                !equation of state specification
FEQ  Helmholtz equation of state for isobutane 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), 0.3% at temperatures
?below 300 K and pressures above 12 MPa, 0.1% in the vapor phase between 340 and
?450 K, and 0.5% elsewhere. In the critical region, deviations in pressure are
?0.5%. Uncertainties in heat capacities are typically 1-2%, rising to 5% in the
?critical region and at temperatures below 200 K. Uncertainties in the speed of
?sound are typically 1-2%, rising to 5% at temperatures below 200 K and in the
?critical region.
?\
!end of info section
113.73                !lower temperature limit [K]
575.0                 !upper temperature limit [K]
35000.0               !upper pressure limit [kPa]
12.9                  !maximum density [mol/L]
CPP                   !pointer to Cp0 model
58.1222               !molecular weight [g/mol]
113.73                !triple point temperature [K]
0.0000219             !pressure at triple point [kPa]
12.74                 !density at triple point [mol/L]
261.401               !normal boiling point temperature [K]
0.184                 !acentric factor
407.81                3629.0          3.879756788 !Tc [K], pc [kPa], rhoc [mol/L]
407.81                3.879756788    !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
.20686820727966D+01    0.5      1.      0      !a(i),t(i),d(i),l(i)
-.36400098615204D+01    1.0      1.      0
.51968754427244D+00    1.5      1.      0
.17745845870123D+00    0.0      2.      0
-.12361807851599D+00    0.5      3.      0
.45145314010528D-01    0.5      4.      0
.30476479965980D-01    0.75     4.      0
.75508387706302D+00    2.0      1.      1
-.85885381015629D+00    2.5      1.      1
.36324009830684D-01    2.5      2.      1
-.19548799450550D-01    1.5      7.      1
-.44452392904960D-02    1.0      8.      1
.46410763666460D-02    1.5      8.      1
-.71444097992825D-01    4.0      1.      2
-.80765060030713D-01    7.0      2.      2
.15560460945053D+00    3.0      3.      2
.20318752160332D-02    7.0      3.      2
-.10624883571689D+00    3.0      4.      2
.39807690546305D-01    1.0      5.      2
.16371431292386D-01    6.0      5.      2
.53212200682628D-03    0.0     10.     2
-.78681561156387D-02    6.0      2.      3
-.30981191888963D-02    13.0     6.      3
-.42276036810382D-01    2.0      1.  2  2  -10.  -150.  1.16  .85  0.  0.  0.
-.53001044558079D-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 EOS of Buecker and Wagner for reference
?\
!end of info section
113.73                    !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
4.05956619      0.00000
4.94641014      387.94064
4.09475197      973.80782
15.6632824      1772.71103
9.73918122      4228.52424

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@EOS                !equation of state specification
FEK  Helmholtz equation of state for isobutane 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
113.73                !lower temperature limit [K]
575.0                 !upper temperature limit [K]
35000.0               !upper pressure limit [kPa]
12.9                  !maximum density [mol/L]
PHK                                !pointer to Cp0 model
58.1222                !molecular weight [g/mol]
113.73                 !triple point temperature [K]
1.                     !pressure at triple point [kPa]
1.                     !density at triple point [mol/L]
261.42                !normal boiling point temperature [K]
0.1841                !acentric factor
407.817                3633.1        3.86014294 !Tc [K], pc [kPa], rhoc [mol/L]
407.817                3.86014294  !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
0.10429331589100d1    0.250  1.  0
-0.28184272548892d1   1.125  1.  0
0.86176232397850     1.500  1.  0
-0.10613619452487     1.375  2.  0
0.98615749302134d-1   0.250  3.  0
0.23948208682322d-3   0.875  7.  0
0.30330004856950     0.625  2.  1
-0.41598156135099d-1   1.750  5.  1
-0.29991937470058     3.625  1.  2
-0.80369342764109d-1   3.625  4.  2
-0.29761373251151d-1  14.5   3.  3
0.13059630303140d-1  12.0   4.  3

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#AUX                !auxiliary model specification
PHK  Helmholtz form for the ideal-gas state for isobutane 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
    3.06714      1.                !ai, ti for [ai*log(tau**ti)] terms
    20.413726078 0.                !aj, ti for [ai*tau**ti] terms
-94.467620036 1.
    -5.25156     0.485556021      !aj, ti for cosh and sinh terms
-16.1388         2.19158348
    8.97575     1.074673199
    25.1423     4.671261865

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#AUX                !auxiliary model specification
PH0  Helmholtz form for the ideal-gas state
?LITERATURE REFERENCE \
?\
!end of info section
113.73              !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))
 3.05956619        1.          !ai, ti for [ai*log(tau**ti)] terms
11.60865546        0.          !aj, ti for [ai*tau**ti] terms
-5.29450411        1.
 4.94641014        -0.9512779015 !aj, ti for [ai*log(1-exp(ti*tau))] terms
 4.09475197        -2.3878958853
15.6632824         -4.3469042691
 9.73918122        -10.3688586351

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@EOS                !equation of state specification
FE1  Helmholtz equation of state for isobutane of Miyamoto and Watanabe (2001).
?LITERATURE REFERENCE \
?Miyamoto, H. and Watanabe, K.
? "A Thermodynamic Property Model for Fluid-Phase Isobutane,"
? Int. J. Thermophys., 23(2):477-499, 2002.
?\
?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
113.56                !lower temperature limit [K]
573.0                 !upper temperature limit [K]
35000.0               !upper pressure limit [kPa]
12.90                 !maximum density [mol/L]
CP1                   !pointer to Cp0 model
58.1222               !molecular weight [g/mol]
113.56                !triple point temperature [K]
0.000021              !pressure at triple point [kPa]
12.738                !density at triple point [mol/L]
261.48                !normal boiling point temperature [K]
0.185                 !acentric factor
407.817               3640.0           3.8601429 !Tc [K], pc [kPa], rhoc [mol/L]
407.817               3.8601429       !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
  2.892737D-1         -0.25      1.0      0 !a(i),t(i),d(i),l(i)
-1.342570D0           1.5        1.0      0
-7.976713D-3          -0.75      2.0      0
  2.025793D-1          0.         2.0      0
-4.241612D-2           1.25      3.0      0
  2.617971D-3          1.5        5.0      0
  5.068955D-5          0.5        8.0      0
-1.144596D-6           2.5        8.0      0
-1.930153D0           1.5        3.0      1
  1.982609D0           1.75      3.0      1
  2.076533D-3          -0.25      8.0      1
-4.958752D-3           3.0        5.0      1
  1.377372D-3           3.0        6.0      1
-1.582662D-1           4.0        1.0      2
-4.961892D-2           2.0        5.0      2
  9.451030D-4          -1.0        7.0      2
-3.037276D-2           2.0        2.0      3
-1.382675D-2          19.0        3.0      3
  8.876254D-5           5.0       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 Isobutane,"
? Int. J. Thermophys., 23(2):477-499, 2002.
?\
!end of info section
113.56              !lower temperature limit [K]
573.0               !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
4.059347           0.00000
4.940314           387.75987
4.090139           972.01102
9.739581           4235.81166
15.68832           1772.81924

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@EOS                !equation of state specification
BWR MBWR equation of state for isobutane 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 density is 0.1%. The uncertainty is
?2% for heat capacities, 0.5% for the speed of sound in the vapor, and 1%
?for the speed of sound in the liquid.
?\
?N.B. all temperatures on IPTS-68
?\
!end of info section
113.55                !lower temperature limit [K]
600.0                !upper temperature limit [K]
35000.0              !upper pressure limit [kPa]
12.89                !maximum density [mol/L]
CP2                  !pointer to Cp0 model
58.1222              !molecular weight [g/mol]
113.55              !triple point temperature [K]
1.948d-5            !pressure at triple point [kPa]
12.755              !density at triple point [mol/L]
261.537            !normal boiling point temperature [K]
0.18534            !acentric factor
407.85              3640.          3.860      !Tc [K], pc [kPa], rhoc [mol/L]
407.85              3.860        !reducing parameters [K, mol/L]
3.860              !gamma
0.0831434          !gas constant [L-bar/mol-K]
    32      1      !Nterm, Ncoeff per term
    0.1307325972d-01  0.3927802742d+00 -0.3185427394d+02
    0.7608825192d+04 -0.1753919859d+07 -0.2090019755d-02
    0.8959557971d+01 -0.6816710130d+04 -0.1111271045d+07
    0.3248737572d-03 -0.1046526456d+01  0.6536598969d+03
    0.3726503734d-01  0.8553649395d+01  0.2109987236d+04
   -0.1401267363d+01  0.5213089327d-01 -0.1925026382d+02
    0.7640067895d+00  0.3425854273d+07 -0.3373475924d+09
    0.1180683444d+06  0.1529683738d+10  0.3323837416d+04
    0.6423169487d+05  0.3891706042d+02 -0.1494755736d+07
   -0.1720240173d-01  0.2894195375d+03  0.2005086329d-02
   -0.4448393005d+00  0.8028488415d+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
113.55              !lower temperature limit [K]
600.0               !upper temperature limit [K]
0.0                !upper pressure limit [kPa]
0.0                !maximum density [mol/L]
1.0                8.31434                !reducing parameters for T, Cp0
  7  1    0  0    0  0  0                !Nterms:  polynomial, exponential, cosh, sinh
  1.7027919006d+7    -3.00d0
 -4.7269724737d+5    -2.00d0
  4.7301406581d+3    -1.00d0
 -1.7231723278d+1     0.00d0
  5.8491344291d-2     1.00d0
  8.9440351886d-6     2.00d0
 -1.8274599197d-8     3.00d0
 -1.9283021962d+1    3000.d0

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@EOS                !equation of state specification
FES  short Helmholtz equation of state for isobutane 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
113.55                !lower temperature limit [K]
600.0                !upper temperature limit [K]
100000.0             !upper pressure limit [kPa]
12.89                !maximum density [mol/L]
CPS                  !pointer to Cp0 model
58.123               !molecular weight [g/mol]
113.55               !triple point temperature [K]
0.000020860          !pressure at triple point [kPa]
12.784               !density at triple point [mol/L]
261.42               !normal boiling point temperature [K]
0.185                !acentric factor
407.817              3640.0          3.8600898 !Tc [K], pc [kPa], rhoc [mol/L]
407.817              3.8600898      !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
  0.104293320000E+01  0.25      1.0      0 !a(i),t(i),d(i),l(i)
-0.281842730000E+01  1.125     1.0      0
  0.861762320000E+00  1.5       1.0      0
-0.106136190000E+00  1.375     2.0      0
  0.986157490000E-01  0.25     3.0      0
  0.239482090000E-03  0.875    7.0      0
  0.303300050000E+00  0.625    2.0      1
-0.415981560000E-01  1.75     5.0      1
-0.299919370000E+00  3.625    1.0      2
-0.803693430000E-01  3.625    4.0      2
-0.297613730000E-01  14.5     3.0      3
  0.130596300000E-01  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
113.55              !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
    0.4067140E+01    0.0
    0.2059196E+06   -2.0    0.1980180E+03   -1.0   -2.0
    0.1289193E+08   -2.0    0.8937650E+03   -1.0   -2.0
    0.1724067E+07   -2.0    0.4382700E+03   -1.0   -2.0
    0.9124395E+08   -2.0    0.1905020E+04   -1.0   -2.0

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@EOS                !equation of state specification
FE3  Helmholtz equation of state for isobutane 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
120.0                !lower temperature limit [K]
498.0                !upper temperature limit [K]
35000.0              !upper pressure limit [kPa]
12.89                !maximum density [mol/L]
CP3                  !pointer to Cp0 model
58.124               !molecular weight [g/mol]
120.0                !triple point temperature [K]
0.46491d-4           !pressure at triple point [kPa]
12.649               !density at triple point [mol/L]
261.51               !normal boiling point temperature [K]
0.1851               !acentric factor
407.85               3640.0           3.8607116 !Tc [K], pc [kPa], rhoc [mol/L]
407.85               3.8607116      !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
-0.958589873652d+0  3.0           0.0       0  0.0           !a(i),t(i),d(i),l(i)
  0.818846326211d+0  4.0           0.0       0  0.0
-0.115814967179d+0  5.0           0.0       0  0.0
  0.345513148715d+0  0.0           1.0       0  0.0
-0.168751721524d+1  1.0           1.0       0  0.0
  0.936693300209d+0  2.0           1.0       0  0.0
-0.106644545724d+1  3.0           1.0       0  0.0
  0.980958295776d-1  4.0           1.0       0  0.0
  0.495941129005d+0  0.0           2.0       0  0.0
-0.261313404262d+0  1.0           2.0       0  0.0
  0.485109471188d+0  2.0           2.0       0  0.0
-0.177275820736d+0  0.0           3.0       0  0.0
-0.209415485311d-1  1.0           3.0       0  0.0
  0.788178884079d-1  0.0           4.0       0  0.0
-0.102751671767d+0  1.0           4.0       0  0.0
  0.178645875838d-1  1.0           5.0       0  0.0
  0.958589873652d+0  3.0           0.0       2  1.0071072
-0.818846326211d+0  4.0           0.0       2  1.0071072
  0.115814967179d+0  5.0           0.0       2  1.0071072
  0.537585249054d+0  3.0           2.0       2  1.0071072
-0.719424468790d+0  4.0           2.0       2  1.0071072
  0.245830118086d+0  5.0           2.0       2  1.0071072

```

```

#AUX                      !auxiliary model specification
CP3  ideal gas heat capacity function
?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
120.0                      !lower temperature limit [K]
498.0                      !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
  0.397893d+00      0.00
  0.412501d-02      1.00
-0.196195d-06      2.00
  0.380185d-08      3.00
-0.523950d-11      4.00

```

```

#TCX          !thermal conductivity model specification
TC1 pure fluid thermal conductivity model of Perkins (2002).
?LITERATURE REFERENCE \
?Perkins, R.A.,
? "Measurement and Correlation of the Thermal Conductivity of Isobutane
? from 114 K to 600 K at Pressures to 70 MPa,"
? J. Chem. Eng. Data, 47(5):1272-1279, 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
113.55          !lower temperature limit [K]
600.0           !upper temperature limit [K]
70000.0         !upper pressure limit [kPa]
13.00          !maximum density [mol/L]
3 0            !# terms for dilute gas function: numerator, denominator
407.85 1.0      !reducing parameters for T, tcx
-2.37901d-3 0.00d0 !coeff, power in T
1.06601d-2 1.00d0
2.15811d-2 2.00d0
10 0           !# terms for background gas function: numerator, denominator
407.85 3.86 1.0 !reducing par for T, rho, tcx
-4.11789d-2 0.0 1.0 0.0 !coeff, powers of T, rho, spare for future use
4.76346d-2 1.00d0 1.00d0 0.00d0
1.46805d-1 0.00d0 2.00d0 0.00d0
-1.28445d-1 1.00d0 2.00d0 0.00d0
-1.19190d-1 0.00d0 3.00d0 0.00d0
1.07565d-1 1.00d0 3.00d0 0.00d0
4.10226d-2 0.00d0 4.00d0 0.00d0
-3.85968d-2 1.00d0 4.00d0 0.00d0
-4.88704d-3 0.00d0 5.00d0 0.00d0
5.20901d-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 (2002).
?LITERATURE REFERENCE \
?Perkins, R.A.,
? "Measurement and Correlation of the Thermal Conductivity of Isobutane
? from 114 K to 600 K at Pressures to 70 MPa,"
? J. Chem. Eng. Data, 47(5):1272-1279, 2002.
?\
!end of info section
113.55              !lower temperature limit [K]
600.0               !upper temperature limit [K]
70000.0             !upper pressure limit [kPa]
13.00               !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) [-]
0.657661d-9         !qd_inverse (modified effective cutoff parameter) [m]
611.73              !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
113.55          !lower temperature limit [K]
600.0           !upper temperature limit [K]
35000.          !upper pressure limit [kPa]
12.90           !maximum density [mol/L]
CI2             !pointer to collision integral model
0.509217        !Lennard-Jones coefficient sigma [nm]
418.0           !Lennard-Jones coefficient epsilon/kappa [K]
 2.0352526600d-01 !const in Eq 19 = 5/16*(k*MW/1000/pi/Na)**0.5*1.0d12
 0.1449797353d+01 !dilute gas terms (Eq 27): Gt(1)
-0.1685643887d+00 ! Gt(2)
 0.4307008989d-02 !residual terms (Eqs 26, 28-30): Et(1)
-0.1509010974d+01
 0.4693712392d+03
-0.3554280979d-03
 0.1841552874d+00
-0.3892338766d+02
-0.9354624917d-01
 0.7114330590d+01 !Et(8)
TK2             !pointer to critical enhancement model (follows immediately)
 0.0034718d0     !critical enhancement terms (Eqs D1-D4): X1
10.1207d0
 0.466392d0
 1.00344d0        !X4
 9.10218d-10      !Z
 1.38054d-23      !Boltzmann's constant, k
 1.6878386520d+0 !coeff for initial density dependence of viscosity (eq 21); Fv(1)
 0.0              !Fv(2)
 1.40             !Fv(3)
 407.85           !Fv(4)
-0.2055498053d+2 !coefficients for residual viscosity, eqs (22 - 25)
 0.1357076181d+4 !Ev(2) (the viscosity is also used in conductivity
correlation)
 0.1893774336d+2 !Ev(3)
-0.1822277344d+5 !Ev(4)
-0.4599387773d-2 !Ev(5)
 0.6305247065d+2 !Ev(6)
 0.1282253921d+5 !Ev(7)

```

```

#ETA                !viscosity model specification
VS1 pure fluid viscosity model of Vogel et al. (2000).
?LITERATURE REFERENCE \
?Vogel, E., Kuechenmeister, C., and Bich, E.,
? "Viscosity Correlation for Isobutane over Wide Ranges of the Fluid Region,"
? Int. J. Thermophys, 21(2):343-356, 2000.
?\
?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
113.55              !lower temperature limit [K]
600.0               !upper temperature limit [K]
35000.0             !upper pressure limit [kPa]
12.90               !maximum density [mol/L]
1                   !number of terms associated with dilute-gas function
CI1                 !pointer to reduced effective collision cross-section model
0.46445             !Lennard-Jones coefficient sigma [nm]
307.55              !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
  307.55 0.0603345   !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
407.817 3.86 1.0    !reducing parameters for T, rho, eta
  0.233859774637D1 0.0 0.00 0.00 0
  0.235255150838D1 0.5 0.00 0.00 0
  0.103511763411D3 0.0 2.00 0.00 0
-0.312670896234D3 -1.0 2.00 0.00 0
  0.145253750239D3 -2.0 2.00 0.00 0
-0.210649894193D3 0.0 3.00 0.00 0
  0.386269696509D3 -1.0 3.00 0.00 0
-0.214963015527D3 -2.0 3.00 0.00 0
  0.112580360920D3 0.0 4.00 0.00 0
-0.223242033154D3 -1.0 4.00 0.00 0
  0.119114788598D3 -2.0 4.00 0.00 0
-0.181909745900D2 0.0 5.00 0.00 0
  0.360438957232D2 -1.0 5.00 0.00 0
-0.213960184050D2 -2.0 5.00 0.00 0
-0.194037606990D4 0.0 1.00 -1.00 0
  0.194037606990D4 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. (2000).
?LITERATURE REFERENCE \
?Vogel, E., Kuechenmeister, C., and Bich, E.,
? "Viscosity Correlation for Isobutane over Wide Ranges of the Fluid Region,"
? Int. J. Thermophys, 21(2):343-356, 2000.
?\
!end of info section
113.55              !lower temperature limit [K]
600.0               !upper temperature limit [K]
0.0                 !(dummy) upper pressure limit
0.0                 !(dummy) maximum density
3                   !number of terms
 0.53583008 0       !coeff, power of Tstar
-0.45629630 1
 0.049911282 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
10%.
?\
?N.B. all temperatures on IPTS-68
?\
!end of info section
113.55          !lower temperature limit [K]
600.0           !upper temperature limit [K]
35000.          !upper pressure limit [kPa]
12.90           !maximum density [mol/L]
CI2             !pointer to collision integral model
0.509217        !Lennard-Jones coefficient sigma [nm]
418.0           !Lennard-Jones coefficient epsilon/kappa [K]
 2.0352526600d-1 !const in Eq 19 = 5/16*(k*MW/1000/pi/Na)**0.5*1.0d12
 0.5            !exponent in Eq 19 for T
 1.6878386520d+0 !coeff for initial density dependence of viscosity (eq 21);
Fv(1)
 0.0            !Fv(2)
 1.40           !Fv(3)
 407.85         !Fv(4)
-0.2055498053d+2 !coefficients for residual viscosity, eqs (22 - 25)
 0.1357076181d+4 !Ev(2)
 0.1893774336d+2 !Ev(3)
-0.1822277344d+5 !Ev(4)
-0.4599387773d-2 !Ev(5)
 0.6305247065d+2 !Ev(6)
 0.1282253921d+5 !Ev(7)
 3.86           !Ev(8)
NUL             !pointer to critical enhancement auxiliary function (none used)

```

```

#AUX                !auxiliary model 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

```

```

@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:
?\
?Vogel, E., Kuechenmeister, C., and Bich, E.,
? "Viscosity Correlation for Isobutane over Wide Ranges of the Fluid Region,"
? Int. J. Thermophys, 21(2):343-356, 2000.
?\
!end of info section
113.55                !lower temperature limit [K]
600.0                !upper temperature limit [K]
35000.0              !upper pressure limit [kPa]
12.90                !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)
0.46445              !Lennard-Jones coefficient sigma [nm]
307.55               !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 of Baidakov and Sulla (1985).
?LITERATURE REFERENCE \
?Baidakov, V.G. and Sulla, I.I.
? "Surface tension of propane and isobutane at near-critical temperatures,"
? Russian Journal of Physical Chemistry, 59:551-554, 1985.
?\
!end of info section
113.73      !lower temperature limit [K]
407.81      !upper temperature limit [K]
0.0         !(dummy) upper pressure limit
0.0         !(dummy) maximum density
2           !number of terms in surface tension model
407.81      !critical temperature used by Baidakov and Sulla
(dummy)
0.05756     1.290      !sigma0 and n
-0.009554   2.290

```



```

#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
0.388417      -1.     1.     0.     !coef, t exp, d exp
20.534        0.     1.     0.
0.020         1.     1.     0.
126.25        0.     2.     0.
52.91         1.     2.     0.
-7501.4       0.     2.9    0.
-2672.9       1.     2.9    0.

```

```
#MLT          !melting line specification
ML1  melting line model of Buecker and Wagner (2005).
?LITERATURE REFERENCE \
? see EOS for reference
?\
!end of info section
113.73          !lower temperature limit [K]
575.0           !upper temperature limit [K]
0.0            !(dummy) upper pressure limit
0.0            !(dummy) maximum density
113.73 0.000022891 !reducing temperature and pressure
2 0 0 0 0 0      !number of terms in melting line equation
-1953637129.    0.      !coefficients and exponents
1953637130.    6.12
```

```
#PS          !vapor pressure equation
PS5  vapor pressure equation of Buecker and Wagner (2005).
?LITERATURE REFERENCE \
?See EOS
?\
!end of info section
113.73        !lower temperature limit [K]
407.81        !upper temperature limit [K]
0.0           !(dummy) upper pressure limit
0.0           !(dummy) maximum density
407.81 3629.0  !reducing parameters
4 0 0 0 0 0   !number of terms in equation
-6.85093103    1.0   !coefficients and exponents
 1.36543198    1.5
-1.32542691    2.5
-2.56190994    4.5
```

```
#DL          !saturated liquid density equation
DL2  saturated liquid density equation of Buecker and Wagner (2005).
?LITERATURE REFERENCE \
?See EOS
?\
!end of info section
113.73          !lower temperature limit [K]
407.81          !upper temperature limit [K]
0.0             ! (dummy) upper pressure limit
0.0             ! (dummy) maximum density
407.81 3.879756788 !reducing parameters
4 0 0 0 0 0          !number of terms in equation
  2.04025104        1.065 !coefficients and exponents
  0.850874089        3.0
-0.479052281        4.0
  0.348201252        7.0
```

```
#DV          !saturated vapor density equation
DV6  saturated vapor density equation of Buecker and Wagner (2005).
?LITERATURE REFERENCE \
?See EOS
?\
!end of info section
113.73          !lower temperature limit [K]
407.81          !upper temperature limit [K]
0.0            !(dummy) upper pressure limit
0.0            !(dummy) maximum density
407.81 3.879756788 !reducing parameters
4 0 0 0 0 0      !number of terms in equation
-2.12933323      1.065 !coefficients and exponents
-2.93790085      2.5
-0.89441086      9.5
-3.46343707      13.0
```

@END

c	1	2	3	4	5	6	7
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8

c23456789012345678901234567890123456789012345678901234567890123456789

0