Supporting Information to

Pure- and Pseudo-Pure Fluid Thermophysical Property Evaluation and the Open-Source Thermophysical Property Library CoolProp

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Industrial & Engineering Chemical Research

Pure and Pseudo-pure fluids

Table 1 presents a listing of the literature sources for the equations of state and transport properties of the pure- and pseudo-pure fluids implemented in CoolProp. If there is no entry for the isobaric ideal-gas specific heat, it has been provided by the publication for the equation of state.

With respect to the transport properties, if a fluid has a fluid-specific correlation for its viscosity and/or thermal conductivity, this correlation is used. If not, extended corresponding states is employed, using the correction polynomial if available.

Most fluids have fluid-specific correlations for their surface tension. If a fluid does not have a fluid specific surface tension correlation, the correlation of Miqueu et al.[1] is used.

Incompressible liquids, aqueous solutions and slurries

Table 2 presents a listing of the incompressible liquids implemented in CoolProp that are derived from the properties from Melinder.[2]

Table 3 presents a listing of the high-temperature incompressible liquids that have been implemented in CoolProp based on curve-fits of manufacturer data. The Nitrate Salt Blend NaK is taken from the work of Zavoico.[3]

Table 4 presents a listing of the aqueous solutions and slurries that have been implemented in CoolProp. The abbreviations that begin with the letter M are taken from Melinder[2], and the others (IceEA, IcePG, IceNA, PK2000, ZiAC) are taken by permission from SecCool, a software package developed by Morten Juel Skovrup of IPU. The aqueous solution of Lithium Bromide in water is modelled according to the equations proposed by Pátek and Klomfar[4] .

Table 1: Literature references of the thermophysical property correlations implemented in CoolProp
EOS: Equation of State
$c_{p,0}$: Ideal-gas specific heat correlation
η : Fluid-specific correlation for viscosity
λ : Fluid-specific correlation for thermal conductivity
L-J : Lennard-Jones parameters
ECS : polynomial correction terms for ECS
σ : Surface Tension

Substance	CAS	EOS	$c_{p,0}$	η	λ	L-J	ECS	σ
1-Butene	106-98-9	5						6
Acetone	67-64-1	7				8		6
Air	N/A	9		10	10			6
Ammonia	7664-41-7	11		12	13			6
Argon	7440-37-1	14		10	10			6
Benzene	71-43-2	15			16	8		6
Carbon Dioxide	124-38-9	17		18	18			6
Carbon Monoxide	630-08-0	7				8		6
Carbonyl Sulfide	463-58-1	7				8		6
Cyclohexane	110-82-7	19	20			21		6
Cyclopropane	75-19-4	22	22					
Cyclopentane	287-92-3	23						
D4	556-67-2	24						6
D5	541-02-6	24						6
D6	540-97-6	25						6
Deuterium	7782-39-0	26						6
Dimethyl Carbonate	616-38-6	27						
Dimethyl Ether	115-10-6	28		29		21		6
Ethane	74-84-0	30		31	31	31		6
Ethanol	64-17-5	32		33	34	33		6
Ethylbenzene	100-41-4	35						
Ethylene	74-85-1	36				8		
Fluorine	7782-41-4	37	37					6
HFE143a	421-14-7	38						
Helium	7440-59-7	39		40	41			6
Hydrogen	1333-74-0	42		43	44	8		6
Hydrogen Sulfide	7783-06-4	7		45		45		6
Isobutane	75-28-5	46		47	48	47		6
Isobutene	115-11-7	5						6
Isohexane	107-83-5	7				21		6
Isopentane	78-78-4	7				21		6
Krypton	7439-90-9	7				8		6
MD2M	141-62-8	25						6
MD3M	141-63-9	25						6
MD4M	107-52-8	24						6
MDM	107-51-7	25						6
MM	107-46-0	24						6
Methane	74-82-8	49						6
Methanol	67-56-1	50						6
Methyl Linoleate	112-63-0	51						
Methyl Linolenate	301-00-8	51						
Methyl Oleate	112-62-9	51						
Methyl Palmitate	112-39-0	51						

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Substance	CAS	EOS	$c_{p,0}$	η	λ	L-J	ECS	σ
Methyl Stearate	112-61-8	51						
Neon	7440-01-9	52				8		6
Neopentane	463-82-1	7				21		
Nitrogen	7727-37-9	53		10	10	8		6
Nitrous Oxide	10024-97-2	7				8		6
Ortho-Deuterium	7782-39-0o	26						
Ortho-Hydrogen	1333-74-0o	42						
Oxygen	7782-44-7	54		10	10			6
Para-Deuterium	7782-39-0p	26						
Para-Hydrogen	1333-74-0p	42			44			6
Propylene	115-07-1	55				56	56	6
Propyne	74-99-7	22	22					
R11	75-69-4	57	58			59		6
R113	76-13-1	60						6
R114	76-14-2	61	61					6
R116	76-16-4	7				56	56	6
R12	75-71-8	60						6
R123	306-83-2	57	62	63	64	63		6
R1234yf	754-12-1	65			66			6
R1234ze(E)	29118-24-9	67			66			
R1234ze(Z)	29118-25-0	68						
R124	2837-89-0	69				56	56	6
R125	354-33-6	70		71	72	71		6
R13	75-72-9	61	61			56	56	6
R134a	811-97-2	73		56	59	56		6
R14	75-73-0	61	61			56	56	6
R141b	1717-00-6	7				56	56	6
R142b	75-68-3	7				56	56	6
R143a	420-46-2	74				59		6
R152a	75-37-6	57	75	76	76			6
R161	353-36-6	77						6
R21	75-43-4	61	61					6
R218	76-19-7	7				56	56	6
R22	75-45-6	78				59	59	6
R227ea	431-89-0	79				56	56	6
R23	75-46-7	80		81	81	81		6
R236ea	431-63-0	82				56	56	6
R236fa	690-39-1	83				56	56	6
R245fa	460-73-1	7				56	56	6
R32	75-10-5	84				56	56	6
R365mfc	406-58-6	79						6
R404A	N/A	85		86	87			88
R407C	N/A	85		86	87			88
R407F	N/A							
R41	593-53-3	7				21		6
R410A	N/A	85		86	87			
R507A	N/A	85		86	87			
RC318	115-25-3	61	61			56	56	6
SES36	N/A	89						
Sulfur Dioxide	7446-09-5	7				8		6
Sulfur Hexafluoride	2551-62-4	90		91	92	91		6
Toluene	108-88-3	7			93			6

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Substance	CAS	EOS	$c_{p,0}$	η	λ	L-J	ECS	σ
Water	7732-18-5	94		95	96	8		6
Xenon	7440-63-3	7				8		6
cis-2-butene	590-18-1	5						
m-Xylene	108-38-3	35						
n-Butane	106-97-8	46		97	98	97		6
n-Decane	124-18-5	7		99	100	99		6
n-Dodecane	112-40-3	101		102	102	102		6
n-Heptane	142-82-5	19	103		104	21		6
n-Hexane	110-54-3	19	103	105	106	8		6
n-Nonane	111-84-2	7		99	100	99		6
n-Octane	111-65-9	19	103	99	100	99		6
n-Pentane	109-66-0	19	103			8		6
n-Propane	74-98-6	107		108	109	21		6
n-Undecane	1120-21-4	110						
o-Xylene	95-47-6	35						
p-Xylene	106-42-3	35						
trans-2-butene	624-64-6	5						

Table 2: Incompressible Liquids from Melinder[2]

Abbreviation	Description
DEB	Diethyl Benzene
HFE	Hydrofluoroether HFE-7100
PMS1	Polydimethylsiloxan 1.
PMS2	Polydimethylsiloxan 2.
SAB	Synthetic alkyl benzene
HCB	Hydrocarbon blend (Dynalene MV)
TCO	Terpene from citrus oils

Table 3: High-temperature secondary working fluids with data from manufacturer

Abbreviation	Description
TD12	Therminol D12 (-85 to +230°C)
TVP1	Therminol VP-1 (+12 to +397°C)
T72	Therminol 72 (-10 to +380°C)
T66	Therminol 66 (0 to +345°C)
DowJ	Dowtherm J (-80 to +345°C)
DowQ	Dowtherm Q (-35 to +360°C)
TX22	Texatherm 22 (0 to +350°C)
NaK	Nitrate Salt Blend (+300 to +600°C)
XLT	Syltherm XLT (-100 to +260°C)
HC10	Dynalene HC-10 (-10 to +218°C)
HC20	Dynalene HC-20 (-20 to +210°C)
HC30	Dynalene HC-30 (-30 to +210°C)
HC40	Dynalene HC-40 (-40 to +200°C)
HC50	Dynalene HC-50 (-50 to +210°C)

Table 4: Aqueous solutions and ice slurries

Abbreviation	Description	max. T	max. mass fraction
MEG	Ethylene Glycol ($C_2H_6O_2$)	+100°C	60 %
MPG	Propylene Glycol ($C_3H_8O_2$)	+100°C	60 %
MEA	Ethyl Alcohol, Ethanol (C_2H_6O)	+40°C	60 %
MMA	Methyl Alcohol, Methanol (CH_4O)	+40°C	60 %
MGL	Glycerol ($C_3H_8O_3$)	+40°C	60 %
MAM	Ammonia (NH_3)	+30°C	30 %
MKC	Potassium Carbonate (K_2CO_3)	+40°C	40 %
MCA	Calcium Chloride ($CaCl_2$)	+40°C	30 %
MMG	Magnesium Chloride ($MgCl_2$)	+40°C	30 %
MNA	Sodium Chloride (NaCl)	+40°C	23 %
MKA	Potassium Acetate (CH_3CO_2K)	+40°C	45 %
MKF	Potassium Formate ($CHKO_2$)	+40°C	48 %
MLI	Lithium Chloride (LiCl)	+40°C	24 %
ZiAC	ZitrecAC (corrosion inhibitor)	100°C	50 %
IceEA	Ethanol-water mixture with slurry ice	-10°C	35 %
IcePG	Propylene glycol-water mixture with slurry ice	-10°C	35 %
IceNA	Sodium chloride-water mixture with slurry ice	-5°C	35 %
PK2000	Pekasol 2000 (Potassium acetate and formate)	100°C	100 %

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