Di-n-propyl ether

Other names:	(n-C3H7)2O
	1,1'-OXYBIS PROPANE
	1,1'-Oxybis[propane]
	1-propoxypropane
	4-Oxaheptane
	Dipropyl ether
	Dipropyl oxide
	Ether, di-n-propyl-
	Propane, 1,1'-oxybis-
	Propyl ether
	UN 2384
	n-Propyl ether
Inchi:	InChI=1S/C6H14O/c1-3-5-7-6-4-2/h3-6H2,1-2H3
InchiKey:	POLCUAVZOMRGSN-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCOCCC
Mol. weight [g/mol]:	102.17
CAS:	111-43-3

Physical Properties

Property code	Value	Unit	Source
af	0.3690		KDB
affp	837.90	kJ/mol	NIST Webbook
basg	810.50	kJ/mol	NIST Webbook
chl	-4028.90 ± 2.10	kJ/mol	NIST Webbook
chl	-4033.10 ± 0.79	kJ/mol	NIST Webbook
dm	1.20	debye	KDB
gf	-105.60	kJ/mol	KDB
hf	-293.10	kJ/mol	KDB
hf	-299.00	kJ/mol	NIST Webbook
hf	-293.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-328.80 ± 0.88	kJ/mol	NIST Webbook
hfl	-333.10 ± 2.10	kJ/mol	NIST Webbook
hfus	12.48	kJ/mol	Joback Method
hvap	35.68	kJ/mol	NIST Webbook
hvap	36.50 ± 1.30	kJ/mol	NIST Webbook
hvap	35.70 ± 0.10	kJ/mol	NIST Webbook

hvap	35.79	kJ/mol	NIST Webbook
ie	9.30 ± 0.03	eV	NIST Webbook
ie	9.32 ± 0.01	eV	NIST Webbook
ie	9.49	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
ie	9.27 ± 0.05	eV	NIST Webbook
log10ws	-1.62		Aqueous Solubility Prediction Method
log10ws	-1.62		Estimated Solubility Method
logp	1.823		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3028.00	kPa	KDB
pc	3028.00 ± 6.00	kPa	NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	656.80		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	664.00		NIST Webbook
ripol	782.00		NIST Webbook
ripol	775.00		NIST Webbook
ripol	768.00		NIST Webbook
ripol	775.00		NIST Webbook
ripol	794.00		NIST Webbook
ripol	773.00		NIST Webbook
ripol	774.00		NIST Webbook
ripol	770.00		NIST Webbook
ripol	770.00		NIST Webbook
ripol	777.00		NIST Webbook

ripol	777.00		NIST Webbook
ripol	766.00		NIST Webbook
ripol	770.00		NIST Webbook
ripol	773.00		NIST Webbook
ripol	769.00		NIST Webbook
ripol	769.00		NIST Webbook
sg	422.50	J/mol×K	NIST Webbook
sl	323.90	J/mol×K	NIST Webbook
tb	362.20	K	NIST Webbook
tb	363.16	K	Isobaric (vapour + liquid + liquid) equilibrium data for (di-n-propyl ether + n-propyl alcohol + water) and (diisopropyl ether + isopropyl alcohol + water) systems at 100 kPa
tb	362.87	K	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
tb	363.23	K	(Liquid + liquid) equilibria of (water + propionic acid + dipropyl ether or diisopropyl ether) at T = 298.2 K
tb	364.20	K	NIST Webbook
tb	363.10	K	NIST Webbook
tb	363.26 ± 0.10	K	NIST Webbook
tb	364.15 ± 0.50	K	NIST Webbook
tb	363.90 ± 1.00	K	NIST Webbook
tb	363.23	K	KDB
tb	363.30 ± 0.50	K	NIST Webbook
tc	530.60	K	KDB
tc	530.60	K	NIST Webbook
tc	530.60 ± 0.30	K	NIST Webbook
tf	147.00	K	KDB
tf	149.95 ± 0.40	K	NIST Webbook
tt	158.36 ± 0.06	K	NIST Webbook
tt	149.40 ± 0.10	K	NIST Webbook
tt	158.36	K	KDB
vc	0.390	m3/kmol	KDB
zc	0.2673370		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.77	J/mol×K	380.01	NIST Webbook
cpg	198.45	J/mol×K	399.98	NIST Webbook
cpg	182.95	J/mol×K	360.00	NIST Webbook
cpg	221.05	J/mol×K	460.01	NIST Webbook
cpg	209.91	J/mol×K	430.05	NIST Webbook
cpl	221.60	J/mol×K	298.15	NIST Webbook
cpl	221.45	J/mol×K	298.15	NIST Webbook
dvisc	0.0003850	Pa×s	299.27	Joback Method
dvisc	0.0008855	Pa×s	239.44	Joback Method
dvisc	0.0002210	Pa×s	359.10	Joback Method
dvisc	0.0002844	Pa×s	329.19	Joback Method
dvisc	0.0016051	Pa×s	209.53	Joback Method
dvisc	0.0005575	Pa×s	269.36	Joback Method
dvisc	0.0035470	Pa×s	179.61	Joback Method
hfust	10.77	kJ/mol	158.40	NIST Webbook
hvapt	34.80	kJ/mol	323.00	NIST Webbook
hvapt	34.43	kJ/mol	363.20	KDB
hvapt	31.31	kJ/mol	363.10	NIST Webbook
hvapt	32.20	kJ/mol	426.00	NIST Webbook
hvapt	32.40	kJ/mol	497.50	NIST Webbook
hvapt	34.60	kJ/mol	341.50	NIST Webbook
hvapt	31.40	kJ/mol	363.00	NIST Webbook
hvapt	35.10	kJ/mol	331.00	NIST Webbook
hvapt	34.50	kJ/mol	359.50	NIST Webbook
hvapt	31.27	kJ/mol	363.22	NIST Webbook
hvapt	35.60	kJ/mol	340.50	NIST Webbook
pvap	42.54	kPa	336.55	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	36.71	kPa	332.57	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	29.35	kPa	326.73	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane

pvap	49.98	kPa	341.15	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	60.00	kPa	346.55	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	57.75	kPa	345.34	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	62.30	kPa	347.55	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	78.97	kPa	354.82	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	89.30	kPa	358.73	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	96.32	kPa	361.18	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	60.00	kPa	346.63	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	101.30	kPa	362.87	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane

pvap	135.50	kPa	373.15	Thermodynamics of binary mixtures containing N-methyl-2-pyrrolidinone VLE measurements for systems with ethers Comparison with the Mod. UNIFAC (Do) and DISQUAC models Predictions for VLE, GE m, HEm and SLE?
pvap	74.10	kPa	353.15	Thermodynamics of binary mixtures containing N-methyl-2-pyrrolidinone VLE measurements for systems with ethers Comparison with the Mod. UNIFAC (Do) and DISQUAC models Predictions for VLE, GE m, HEm and SLE?
pvap	84.25	kPa	356.85	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
pvap	72.36	kPa	352.11	Vapor Liquid Equilibria Measurements for Di-n-Propyl Ether and Butyl Ethyl Ether with n-Heptane
rfi	1.37840		298.15	Isobaric vapor-liquid equilibria for the binary systems 1-propyl alcohol + dipropyl ether and 1-butyl alcohol + dibutyl ether at 20 and 101.3 kPa

rfi	1.37840		298.15	Phase Equilibria Involved in Extractive Distillation of Dipropyl Ether + 1-Propyl Alcohol Using N,N-Dimethylformamide as Entrainer
rfi	1.37840		298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Dipropyl Ether, 1-Propyl Alcohol, and Butyl Propionate
rfi	1.37840		298.15	Liquid liquid equilibria of the systems dipropyl ether + n-propanol +water and dipropyl ether + n-propanol + ethylene glycol at different temperatures
rfi	1.37840		298.15	Phase equilibria involved in extractive distillation of dipropyl ether + 1-propyl alcohol using 2-ethoxyethanol as entrainer
rfi	1.37840		298.15	Vapor liquid equilibria in the ternary system dipropyl ether + 1-propanol + 1-pentanol and the binary systems dipropyl ether + 1-pentanol, 1-propanol + 1-pentanol at 101.3 kPa
rhol	736.00	kg/m3	293.00	KDB
rhol	713.73	kg/m3	328.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K

rhol	727.87	kg/m3	313.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rhol	741.94	kg/m3	298.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rhol	699.61	kg/m3	343.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rhol	684.92	kg/m3	358.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rhol	741.98	kg/m3	298.15	Excess molar enthalpies of ternary mixtures (dibutyl ether or dipropyl ether + 2,2-dimethylbutane + 2,3-dimethylbutane) at the temperature 298.15 K
rhol	742.00	kg/m3	298.15	Excess Molar Enthalpies of Dipropyl Ether + Dibutyl Ether + (1-Hexene or Tetrahydrofuran) at 298.15 K
srf	0.02	N/m	298.20	KDB
svapt	86.10	J/mol×K	363.22	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53894e+01
Coeff. B	-3.45615e+03
Coeff. C	-4.21280e+01
Temperature range (K), min.	270.98
Temperature range (K), max.	385.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.93819e+01
Coeff. B	-7.55859e+03
Coeff. C	-1.27960e+01
Coeff. D	1.12163e-05
Temperature range (K), min.	149.95
Temperature range (K), max.	530.60

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	757.39
288.15	100.00	752.52
293.15	100.00	747.63
298.15	100.00	742.71
303.15	100.00	737.77
308.15	100.00	732.8
313.15	100.00	727.8
318.15	100.00	722.77
323.15	100.00	717.7

328.15	100.00	712.59
333.15	100.00	707.45
283.15	5000.00	762.38
288.15	5000.00	757.69
293.15	5000.00	752.98
298.15	5000.00	748.24
303.15	5000.00	743.49
308.15	5000.00	738.69
313.15	5000.00	733.9
318.15	5000.00	729.04
323.15	5000.00	724.25
328.15	5000.00	719.28
333.15	5000.00	714.57
283.15	10000.00	767.05
288.15	10000.00	762.5
293.15	10000.00	757.94
298.15	10000.00	753.37
303.15	10000.00	748.78
308.15	10000.00	744.18
313.15	10000.00	739.57
318.15	10000.00	735.01
323.15	10000.00	730.31
328.15	10000.00	725.68
333.15	10000.00	721.03
283.15	15000.00	771.45
288.15	15000.00	767.01
293.15	15000.00	762.58
298.15	15000.00	758.15
303.15	15000.00	753.68
308.15	15000.00	749.22
313.15	15000.00	744.77
318.15	15000.00	740.33
323.15	15000.00	735.84
328.15	15000.00	731.37
333.15	15000.00	726.88
283.15	20000.00	775.62
288.15	20000.00	771.21
293.15	20000.00	766.89
298.15	20000.00	762.57
303.15	20000.00	758.26
308.15	20000.00	753.95
313.15	20000.00	749.62
318.15	20000.00	745.32
323.15	20000.00	741.0

328.15	20000.00	736.67
333.15	20000.00	732.34
283.15	25000.00	779.52
288.15	25000.00	775.22
293.15	25000.00	771.01
298.15	25000.00	766.81
303.15	25000.00	762.61
308.15	25000.00	758.41
313.15	25000.00	754.2
318.15	25000.00	750.04
323.15	25000.00	745.84
328.15	25000.00	741.66
333.15	25000.00	737.47
283.15	30000.00	783.28
288.15	30000.00	779.05
293.15	30000.00	774.94
298.15	30000.00	770.85
303.15	30000.00	766.76
308.15	30000.00	762.65
313.15	30000.00	758.55
318.15	30000.00	754.51
323.15	30000.00	750.43
328.15	30000.00	746.37
333.15	30000.00	742.3
283.15	35000.00	786.9
288.15	35000.00	782.73
293.15	35000.00	778.69
298.15	35000.00	774.71
303.15	35000.00	770.7
308.15	35000.00	766.7
313.15	35000.00	762.71
318.15	35000.00	758.76
323.15	35000.00	754.79
328.15	35000.00	750.85
333.15	35000.00	746.89
283.15	40000.00	790.38
288.15	40000.00	786.26
293.15	40000.00	782.3
298.15	40000.00	778.42
303.15	40000.00	774.48
308.15	40000.00	770.6
313.15	40000.00	766.68
318.15	40000.00	762.84
323.15	40000.00	758.96

328.15	40000.00	755.1
333.15	40000.00	751.24
283.15	45000.00	793.67
288.15	45000.00	789.68
293.15	45000.00	785.81
298.15	45000.00	781.98
303.15	45000.00	778.13
308.15	45000.00	774.31
313.15	45000.00	770.47
318.15	45000.00	766.72
323.15	45000.00	762.93
328.15	45000.00	759.16
333.15	45000.00	755.35
283.15	50000.00	796.87
288.15	50000.00	792.99
293.15	50000.00	789.18
298.15	50000.00	785.42
303.15	50000.00	781.64
308.15	50000.00	777.92
313.15	50000.00	774.17
318.15	50000.00	770.47
323.15	50000.00	766.76
328.15	50000.00	763.06
333.15	50000.00	759.32
283.15	55000.00	800.02
288.15	55000.00	796.16
293.15	55000.00	792.44
298.15	55000.00	788.74
303.15	55000.00	785.01
308.15	55000.00	781.37
313.15	55000.00	777.67
318.15	55000.00	774.07
323.15	55000.00	770.41
328.15	55000.00	766.79
333.15	55000.00	763.16
283.15	60000.00	802.99
288.15	60000.00	799.26
293.15	60000.00	795.56
298.15	60000.00	791.97
303.15	60000.00	788.28
308.15	60000.00	784.7
313.15	60000.00	781.06
318.15	60000.00	777.53
323.15	60000.00	773.95

328.15	60000.00	770.38
333.15	60000.00	766.84
283.15	65000.00	805.87
288.15	65000.00	802.29
293.15	65000.00	798.64
298.15	65000.00	795.06
303.15	65000.00	791.45
308.15	65000.00	787.86
313.15	65000.00	784.29
318.15	65000.00	780.73
323.15	65000.00	777.21
328.15	65000.00	773.71
333.15	65000.00	770.23

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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility