

n-Amyl ether

Other names:	(n-C5H11)2O 1,1'-OXYBISPENTANE 1-(Pentyloxy)pentane 1-pentoxypentane 6-oxaundecane Amyl ether DI-N-AMYLETHER Di-n-amyl ether Di-n-pentyl ether Diamyl ether Dipentyl ether Ether, di-n-pentyl- NSC 6571 PENTYL ETHER Pentane, 1,1'-oxybis- Pentyloxypentane n-Pentyl ether
Inchi:	InChI=1S/C10H22O/c1-3-5-7-9-11-10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	AOPDRZXCEAKHHW-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCOCCCC
Mol. weight [g/mol]:	158.28
CAS:	693-65-2

Physical Properties

Property code	Value	Unit	Source
affp	852.70	kJ/mol	NIST Webbook
basg	818.40 ± 0.70	kJ/mol	NIST Webbook
basg	819.00	kJ/mol	NIST Webbook
basg	819.00	kJ/mol	NIST Webbook
basg	819.00	kJ/mol	NIST Webbook
basg	825.30	kJ/mol	NIST Webbook
chl	-6644.00 ± 3.00	kJ/mol	NIST Webbook
gf	-71.68	kJ/mol	Joback Method
hf	-390.00	kJ/mol	NIST Webbook
hfl	-435.20 ± 3.00	kJ/mol	NIST Webbook
hfus	22.84	kJ/mol	Joback Method

hvap	40.26	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.383		Crippen Method
mcpvol	157.630	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1069.70		NIST Webbook
rinpol	1069.70		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1165.00		NIST Webbook
tb	459.90 ± 0.07	K	NIST Webbook
tb	460.65 ± 0.40	K	NIST Webbook
tb	460.70	K	NIST Webbook
tb	460.65	K	KDB
tb	459.00	K	NIST Webbook
tb	411.20 ± 0.20	K	NIST Webbook
tc	613.22	K	Joback Method
tf	203.85 ± 0.40	K	NIST Webbook
tf	204.15 ± 0.20	K	NIST Webbook
tf	203.72 ± 0.05	K	NIST Webbook
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.40	J/mol×K	450.62	Joback Method
cpg	357.17	J/mol×K	477.72	Joback Method
cpg	371.45	J/mol×K	504.82	Joback Method
cpg	385.25	J/mol×K	531.92	Joback Method
cpg	398.57	J/mol×K	559.02	Joback Method
cpg	411.42	J/mol×K	586.12	Joback Method
cpg	423.80	J/mol×K	613.22	Joback Method
dvisc	0.0002026	Pa×s	450.62	Joback Method
dvisc	0.0018076	Pa×s	262.35	Joback Method
dvisc	0.0009367	Pa×s	300.00	Joback Method
dvisc	0.0005620	Pa×s	337.65	Joback Method
dvisc	0.0043485	Pa×s	224.69	Joback Method
dvisc	0.0002676	Pa×s	412.97	Joback Method
dvisc	0.0003736	Pa×s	375.31	Joback Method
hvapt	46.20	kJ/mol	416.50	NIST Webbook
hvapt	45.60	kJ/mol	451.50	NIST Webbook
rho1	778.96	kg/m3	298.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rho1	768.65	kg/m3	313.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rho1	756.32	kg/m3	328.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rho1	743.97	kg/m3	343.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K

rhoI	731.37	kg/m3	358.15	Volumetric properties of (N,N-dimethylformamide + aliphatic diethers) at Temperatures ranging from (298.15 to 358.15) K
rhoI	779.10	kg/m3	298.15	Excess molar enthalpies of binary mixtures containing 2-decanone or dipentyl ether with long-chain n-alkanes at T = 298.15 K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53823e+01
Coeff. B	-4.21621e+03
Coeff. C	-6.90020e+01
Temperature range (K), min.	348.32
Temperature range (K), max.	487.66

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	7.06135e+01
Coeff. B	-8.24305e+03
Coeff. C	-7.98994e+00
Coeff. D	4.35446e-06
Temperature range (K), min.	203.72
Temperature range (K), max.	622.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	790.99
288.15	100.00	786.98
293.15	100.00	782.96
298.15	100.00	778.94
303.15	100.00	774.9
308.15	100.00	770.87
313.15	100.00	766.82
318.15	100.00	762.76
323.15	100.00	758.69
328.15	100.00	754.6
333.15	100.00	750.51
283.15	5000.00	794.85
288.15	5000.00	790.95
293.15	5000.00	787.04
298.15	5000.00	783.12
303.15	5000.00	779.22
308.15	5000.00	775.29
313.15	5000.00	771.35
318.15	5000.00	767.42
323.15	5000.00	763.48
328.15	5000.00	759.51
333.15	5000.00	755.54
283.15	10000.00	798.47
288.15	10000.00	794.65
293.15	10000.00	790.83
298.15	10000.00	787.02
303.15	10000.00	783.2
308.15	10000.00	779.38
313.15	10000.00	775.57
318.15	10000.00	771.74
323.15	10000.00	767.94
328.15	10000.00	764.08
333.15	10000.00	760.26
283.15	15000.00	801.9
288.15	15000.00	798.17
293.15	15000.00	794.44
298.15	15000.00	790.73
303.15	15000.00	787.0
308.15	15000.00	783.28

313.15	15000.00	779.56
318.15	15000.00	775.84
323.15	15000.00	772.13
328.15	15000.00	768.39
333.15	15000.00	764.69
283.15	20000.00	805.2
288.15	20000.00	801.55
293.15	20000.00	797.91
298.15	20000.00	794.27
303.15	20000.00	790.65
308.15	20000.00	787.0
313.15	20000.00	783.37
318.15	20000.00	779.77
323.15	20000.00	776.12
328.15	20000.00	772.51
333.15	20000.00	768.87
283.15	25000.00	808.38
288.15	25000.00	804.81
293.15	25000.00	801.23
298.15	25000.00	797.69
303.15	25000.00	794.13
308.15	25000.00	790.57
313.15	25000.00	787.03
318.15	25000.00	783.5
323.15	25000.00	779.95
328.15	25000.00	776.42
333.15	25000.00	772.87
283.15	30000.00	811.47
288.15	30000.00	807.94
293.15	30000.00	804.44
298.15	30000.00	800.97
303.15	30000.00	797.48
308.15	30000.00	793.99
313.15	30000.00	790.53
318.15	30000.00	787.08
323.15	30000.00	783.62
328.15	30000.00	780.18
333.15	30000.00	776.68
283.15	35000.00	814.44
288.15	35000.00	810.97
293.15	35000.00	807.54
298.15	35000.00	804.13
303.15	35000.00	800.72
308.15	35000.00	797.3

313.15	35000.00	793.9
318.15	35000.00	790.52
323.15	35000.00	787.13
328.15	35000.00	783.75
333.15	35000.00	780.35
283.15	40000.00	817.31
288.15	40000.00	813.93
293.15	40000.00	810.53
298.15	40000.00	807.2
303.15	40000.00	803.84
308.15	40000.00	800.48
313.15	40000.00	797.15
318.15	40000.00	793.82
323.15	40000.00	790.51
328.15	40000.00	787.17
333.15	40000.00	783.87
283.15	45000.00	820.12
288.15	45000.00	816.78
293.15	45000.00	813.44
298.15	45000.00	810.16
303.15	45000.00	806.86
308.15	45000.00	803.56
313.15	45000.00	800.28
318.15	45000.00	797.02
323.15	45000.00	793.75
328.15	45000.00	790.5
333.15	45000.00	787.29
283.15	50000.00	822.84
288.15	50000.00	819.54
293.15	50000.00	816.26
298.15	50000.00	813.04
303.15	50000.00	809.78
308.15	50000.00	806.55
313.15	50000.00	803.33
318.15	50000.00	800.1
323.15	50000.00	796.9
328.15	50000.00	793.7
333.15	50000.00	790.54
283.15	55000.00	825.48
288.15	55000.00	822.24
293.15	55000.00	819.01
298.15	55000.00	815.82
303.15	55000.00	812.62
308.15	55000.00	809.43

313.15	55000.00	806.26
318.15	55000.00	803.09
323.15	55000.00	799.95
328.15	55000.00	796.82
333.15	55000.00	793.66
283.15	60000.00	828.06
288.15	60000.00	824.87
293.15	60000.00	821.67
298.15	60000.00	818.54
303.15	60000.00	815.39
308.15	60000.00	812.24
313.15	60000.00	809.11
318.15	60000.00	806.0
323.15	60000.00	802.89
328.15	60000.00	799.82
333.15	60000.00	796.72
283.15	65000.00	830.58
288.15	65000.00	827.41
293.15	65000.00	824.26
298.15	65000.00	821.19
303.15	65000.00	818.05
308.15	65000.00	814.95
313.15	65000.00	811.88
318.15	65000.00	808.83
323.15	65000.00	805.77
328.15	65000.00	802.72
333.15	65000.00	799.67

Reference <https://www.doi.org/10.1016/j.fluid.2016.02.009>

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693652&Units=SI
Volumetric properties of (N,N-dimethylformamide + aliphatic ketones) at temperatures ranging from 283.15 to 338.15 K: binary mixtures containing 2-decanone or diphenyl ether with long-chain n-alkanes at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.01.002 https://www.doi.org/10.1016/j.jct.2010.11.004
KDB Vapor Pressure Data:	https://en.wikipedia.org/wiki/Joback_method https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1023
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1023.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Pure (Korean Thermophysical Properties Databank):
Experimental and modeled volumetric behavior of linear and branched ethers:
Experimental liquid liquid equilibria of 1-methylimidazole with hydrocarbons and ethers:
Solubility of Imidazoles in Ethers:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1023>

<https://www.doi.org/10.1016/j.fluid.2016.02.009>

<https://www.doi.org/10.1016/j.fluid.2005.09.021>

<https://www.doi.org/10.1021/je020113t>

(Solid + liquid) phase equilibria of binary mixtures containing
N-methyl-2-pyrrolidinone and ethers at atmospheric pressure:

<https://www.doi.org/10.1016/j.fluid.2004.11.006>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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