5-Nonanone

Other names:	(n-C4H9)2CO
	5-Oxononane
	Butyl ketone
	DI-N-BUTYL KETONE
	Dibutyl ketone
	Nonan-5-one
	di-n-Butylketone
Inchi:	InChI=1S/C9H18O/c1-3-5-7-9(10)8-6-4-2/h3-8H2,1-2H3
InchiKey:	WSGCRAOTEDLMFQ-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCCC(=O)CCCC
Mol. weight [g/mol]:	142.24
CAS:	502-56-7

Physical Properties

Property code	Value	Unit	Source
affp	853.70	kJ/mol	NIST Webbook
basg	821.90	kJ/mol	NIST Webbook
chl	-5715.80 ± 1.20	kJ/mol	NIST Webbook
gf	-104.02	kJ/mol	Joback Method
hf	-344.90 ± 1.30	kJ/mol	NIST Webbook
hfl	-398.20 ± 1.30	kJ/mol	NIST Webbook
hfus	20.66	kJ/mol	Joback Method
hvap	55.00	kJ/mol	NIST Webbook
hvap	54.90 ± 0.40	kJ/mol	NIST Webbook
hvap	53.30 ± 0.08	kJ/mol	NIST Webbook
hvap	53.30 ± 0.10	kJ/mol	NIST Webbook
hvap	40.20	kJ/mol	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
log10ws	-2.58		Estimated Solubility Method
log10ws	-2.59		Aqueous Solubility Prediction Method
logp	2.936		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method

rhoc	254.61 ± 2.84	kg/m3	NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1076.90		NIST Webbook
rinpol	1076.20		NIST Webbook
rinpol	1074.50		NIST Webbook
rinpol	1073.10		NIST Webbook
rinpol	1075.30		NIST Webbook
rinpol	1051.40		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1077.60		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1353.90		NIST Webbook
ripol	1334.10		NIST Webbook
ripol	1340.60		NIST Webbook
ripol	1353.90		NIST Webbook
ripol	1330.00		NIST Webbook

ripol	1325.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1347.30		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1325.60		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1309.90		NIST Webbook
sl	401.40	J/mol×K	NIST Webbook
tb	459.70	K	NIST Webbook
tb	461.60	K	NIST Webbook
tb	461.10 ± 1.00	K	NIST Webbook
tb	459.00 ± 7.00	K	NIST Webbook
tb	461.00 ± 6.00	K	NIST Webbook
tb	455.00 ± 4.00	K	NIST Webbook
tb	460.80 ± 0.30	K	NIST Webbook
tb	461.90 ± 4.00	K	NIST Webbook
tb	463.00 ± 7.00	K	NIST Webbook
tc	640.00 ± 4.00	K	NIST Webbook
tc	641.40 ± 0.30	K	NIST Webbook
tf	268.35 ± 1.50	K	NIST Webbook
tf	267.30 ± 1.50	K	NIST Webbook
tf	238.55	K	Aqueous Solubility Prediction Method
tt	269.31 ± 0.05	K	NIST Webbook
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.72	J/mol×K	459.19	Joback Method
cpg	311.23	J/mol×K	488.21	Joback Method
cpg	324.21	J/mol×K	517.23	Joback Method
cpg	336.66	J/mol×K	546.25	Joback Method
cpg	348.60	J/mol×K	575.27	Joback Method
cpg	360.04	J/mol×K	604.29	Joback Method
cpg	370.99	J/mol×K	633.31	Joback Method
cpl	306.30	J/mol×K	298.15	NIST Webbook
cpl	303.60	J/mol×K	298.15	NIST Webbook

cpl	303.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0045015	Pa×s	241.12	Joback Method
dvisc	0.0020994	Pa×s	277.47	Joback Method
dvisc	0.0002834	Pa×s	459.19	Joback Method
dvisc	0.0003685	Pa×s	422.85	Joback Method
dvisc	0.0005036	Pa×s	386.50	Joback Method
dvisc	0.0007343	Pa×s	350.15	Joback Method
dvisc	0.0011683	Pa×s	313.81	Joback Method
hfust	11.27	kJ/mol	451.80	NIST Webbook
hfust	11.27	kJ/mol	451.80	NIST Webbook
hfust	24.94	kJ/mol	269.30	NIST Webbook
hvapt	44.70	kJ/mol	464.50	NIST Webbook
hvapt	49.70	kJ/mol	412.50	NIST Webbook
pvap	0.73	kPa	332.32	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.64	kPa	329.95	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.48	kPa	324.99	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.35	kPa	320.18	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.25	kPa	315.00	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.18	kPa	310.19	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.13	kPa	305.38	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.09	kPa	300.56	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.07	kPa	295.75	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	290.90	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.55	kPa	327.44	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.03	kPa	283.83	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	288.55	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	293.35	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	298.10	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.11	kPa	302.92	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.16	kPa	307.75	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.22	kPa	312.99	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.30	kPa	317.81	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.41	kPa	322.62	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.55	kPa	327.49	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.73	kPa	332.35	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.95	kPa	337.15	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.83	kPa	334.71	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.63	kPa	329.90	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.47	kPa	325.05	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.35	kPa	320.16	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.26	kPa	315.38	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.41	kPa	322.58	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.30	kPa	317.80	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.22	kPa	313.02	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.03	kPa	283.85	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.11	kPa	302.94	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	298.12	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	293.32	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	288.55	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.03	kPa	286.19	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.84	kPa	334.74	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.96	kPa	337.13	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.16	kPa	307.77	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
sfust	92.59	J/mol×K	269.30	NIST Webbook
sfust	24.94	J/mol×K	451.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54166e+01
Coeff. B	-4.19534e+03
Coeff. C	-6.94750e+01
Temperature range (K), min.	346.78
Temperature range (K), max.	484.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.69946e+02
Coeff. B	-1.28651e+04
Coeff. C	-2.29607e+01
Coeff. D	1.59500e-05
Temperature range (K), min.	276.15
Temperature range (K), max.	485.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB: https://www.cheric.org/files/research/kdb/mol/mol1212.mol

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation: https://www.doi.org/10.1016/j.fluid.2014.11.026

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1212

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C502567&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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