3-Nonanone

Other names:	Ethyl hexyl ketone
	Ethyl n-hexyl ketone
	n-Hexyl ethyl ketone
	nonan-3-one
Inchi:	InChI=1S/C9H18O/c1-3-5-6-7-8-9(10)4-2/h3-8H2,1-2H3
InchiKey:	IYTXKIXETAELAV-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCCCCC(=O)CC
Mol. weight [g/mol]:	142.24
CAS:	925-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-104.02	kJ/mol	Joback Method
hf	-341.67	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hvap	56.60 ± 0.60	kJ/mol	NIST Webbook
hvap	56.40	kJ/mol	NIST Webbook
hvap	56.40 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.87		Crippen 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	1091.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1362.00		NIST Webbook

ripol	1362.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1362.00		NIST Webbook
tb	459.00 ± 4.00	K	NIST Webbook
tb	461.50 ± 1.50	K	NIST Webbook
tb	460.70	K	NIST Webbook
tc	648.10 ± 0.25	K	NIST Webbook
tf	265.00 ± 4.00	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
dvisc	0.0020994	Pa×s	277.47	Joback Method
dvisc	0.0045015	Pa×s	241.12	Joback Method
dvisc	0.0011683	Pa×s	313.81	Joback Method
dvisc	0.0007343	Pa×s	350.15	Joback Method
dvisc	0.0005036	Pa×s	386.50	Joback Method
dvisc	0.0003685	Pa×s	422.85	Joback Method
dvisc	0.0002834	Pa×s	459.19	Joback Method
hvapt	55.60	kJ/mol	369.50	NIST Webbook
hvapt	52.60	kJ/mol	401.50	NIST Webbook
hvapt	52.70	kJ/mol	386.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53074e+01
Coeff. B	-4.17721e+03
Coeff. C	-6.99060e+01
Temperature range (K), min.	348.02
Temperature range (K), max.	487.80

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C925780&Units=SI

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

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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: 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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume