

2-Nonanone

Other names:	Heptyl methyl ketone Ketone, heptyl methyl METHYL-N-HEPTYL KETONE Methyl heptyl ketone Methyl n-heptyl ketone NONANONE-2 Nonan-2-one n-C7H15COCH3 «beta»-Nonanone Â«betaÂ»-Nonanone
Inchi:	InChI=1S/C9H18O/c1-3-4-5-6-7-8-9(2)10/h3-8H2,1-2H3
InchiKey:	VKCYHJWLYTUGCC-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCCCCCC(C)=O
Mol. weight [g/mol]:	142.24
CAS:	821-55-6

Physical Properties

Property code	Value	Unit	Source
chl	-5716.80 ± 1.20	kJ/mol	NIST Webbook
gf	-104.02	kJ/mol	Joback Method
hf	-340.80 ± 1.70	kJ/mol	NIST Webbook
hfl	-397.20 ± 1.70	kJ/mol	NIST Webbook
hfus	27.35	kJ/mol	Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol)
hvap	56.44 ± 0.06	kJ/mol	NIST Webbook
ie	9.38	eV	NIST Webbook
ie	9.32 ± 0.02	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
log10ws	-2.58		Estimated Solubility Method
log10ws	-2.58		Aqueous Solubility Prediction Method
logp	2.936		Crippen Method

mcvol	139.240	ml/mol	McGowan Method
pc	2482.00 ± 10.00	kPa	NIST Webbook
rhoc	254.61 ± 3.56	kg/m3	NIST Webbook
rinpol	1089.00		NIST Webbook
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tb	464.65 ± 2.00	K	NIST Webbook
tb	468.50	K	NIST Webbook
tb	468.15 ± 2.00	K	NIST Webbook
tb	467.15 ± 2.00	K	NIST Webbook
tb	467.55 ± 2.00	K	NIST Webbook
tb	461.65 ± 2.00	K	NIST Webbook
tb	467.15 ± 2.00	K	NIST Webbook
tb	473.15 ± 2.00	K	NIST Webbook
tb	468.45 ± 2.00	K	NIST Webbook
tc	652.50 ± 0.25	K	NIST Webbook
tc	651.90 ± 0.20	K	NIST Webbook
tf	205.90 ± 0.40	K	NIST Webbook
tf	262.98	K	Aqueous Solubility Prediction Method
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	0.0045015	Pa×s	241.12	Joback Method
dvisc	0.0020994	Pa×s	277.47	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.20	K	99.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50095e+01
Coeff. B	-4.12511e+03
Coeff. C	-7.10180e+01
Temperature range (K), min.	351.22
Temperature range (K), max.	496.37

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.28514e+02
Coeff. B	-1.12636e+04
Coeff. C	-1.65872e+01
Coeff. D	9.99868e-06
Temperature range (K), min.	335.15
Temperature range (K), max.	468.15

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821556&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1211
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1211.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurements, Correlations, and Mod.	https://www.doi.org/10.1021/je100725a
UNIFAC (Do) Prediction of	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Griffin Method	https://www.doi.org/10.1016/j.jct.2010.07.013
Diagrams in Binary Systems (Aliphatic	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Solubility of fragrance raw materials in	
water: Experimental study,	
Conversions, and Mod. UNIFAC (Do)	
predictions:	

Legend

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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