4-Nonanone

Other names: Nonan-4-one
Propyl amyl ketone
Inchi: InChI=1S/C9H18O/c1-3-5-6-8-9(10)7-4-2/h3-8H2,1-2H3
InchiKey: TYBCSQFBSWACAA-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCCC(=O)CCC
Mol. weight [g/mol]: 142.24
CAS: 4485-09-0

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	42.37	kJ/mol	Joback Method
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	1030.00		NIST Webbook
rinpol	1053.00		NIST Webbook
ripol	1356.50		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1390.00		NIST Webbook
tb	460.70	K	NIST Webbook
tb	461.00 ± 4.00	K	NIST Webbook
tc	643.70 ± 0.30	K	NIST Webbook
tf	241.12	K	Joback 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	348.70	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50716e+01
Coeff. B	-4.09236e+03
Coeff. C	-6.92110e+01
Temperature range (K), min.	346.02
Temperature range (K), max.	488.50

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4485090&Units=SI

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
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