

# 4-Decanone

<b>Other names:</b>	Hexyl propyl ketone Propyl hexyl ketone decan-1-oyl chloride n-Propyl n-hexyl ketone
<b>Inchi:</b>	InChI=1S/C10H20O/c1-3-5-6-7-9-10(11)8-4-2/h3-9H2,1-2H3
<b>InchiKey:</b>	MKJDUHZPLQYUCB-UHFFFAOYSA-N
<b>Formula:</b>	C10H20O
<b>SMILES:</b>	CCCCCCC(=O)CCC
<b>Mol. weight [g/mol]:</b>	156.27
<b>CAS:</b>	624-16-8

## Physical Properties

Property code	Value	Unit	Source
gf	-95.60	kJ/mol	Joback Method
hf	-362.31	kJ/mol	Joback Method
hfus	23.25	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.326		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rhoc	248.46 ± 6.25	kg/m3	NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1163.00		NIST Webbook
tb	479.00 ± 5.00	K	NIST Webbook
tb	479.70	K	NIST Webbook
tc	662.90 ± 0.50	K	NIST Webbook
tf	263.90 ± 4.00	K	NIST Webbook
vc	0.602	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/molxK	482.07	Joback Method
cpg	356.42	J/molxK	510.87	Joback Method
cpg	370.27	J/molxK	539.66	Joback Method
cpg	383.54	J/molxK	568.46	Joback Method
cpg	396.27	J/molxK	597.26	Joback Method
cpg	408.46	J/molxK	626.06	Joback Method
cpg	420.12	J/molxK	654.85	Joback Method
dvisc	0.0045381	Paxs	252.39	Joback Method
dvisc	0.0020766	Paxs	290.67	Joback Method
dvisc	0.0011399	Paxs	328.95	Joback Method
dvisc	0.0007090	Paxs	367.23	Joback Method
dvisc	0.0004824	Paxs	405.51	Joback Method
dvisc	0.0003508	Paxs	443.79	Joback Method
dvisc	0.0002683	Paxs	482.07	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	1.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50989e+01
Coeff. B	-4.24681e+03
Coeff. C	-7.44930e+01
Temperature range (K), min.	361.22
Temperature range (K), max.	508.40

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C624168&Units=SI>

**The Yaws Handbook of Vapor**

**Pressure:**

**Crippen Method:**

**Crippen Method:**

**Joback Method:**

**McGowan Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhoc:</b>	Critical density
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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