

2-Decanone

Other names:	Decan-2-one Methyl n-octyl ketone Methyl octyl ketone Octyl methyl ketone n-C8H17COCH3
Inchi:	InChI=1S/C10H20O/c1-3-4-5-6-7-8-9-10(2)11/h3-9H2,1-2H3
InchiKey:	ZAJNGDIORYACQU-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCCCCCC(C)=O
Mol. weight [g/mol]:	156.27
CAS:	693-54-9

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	60.90 ± 0.50	kJ/mol	NIST Webbook
log10ws	-3.30		Estimated Solubility Method
log10ws	-3.31		Aqueous Solubility Prediction Method
logp	3.326		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rhoc	250.02 ± 0.63	kg/m3	NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1188.00		NIST Webbook

rinpol	1169.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1194.00	NIST Webbook
rinpol	1193.00	NIST Webbook
rinpol	1192.00	NIST Webbook
rinpol	1194.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1192.00	NIST Webbook
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rinpol	1198.00	NIST Webbook
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rinpol	1171.00	NIST Webbook
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rinpol	1169.30	NIST Webbook
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rinpol	1171.10	NIST Webbook
rinpol	1192.70	NIST Webbook
rinpol	1179.00	NIST Webbook
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ripol	1494.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	483.15 ± 2.00	K	NIST Webbook

tb	488.00 ± 5.00	K	NIST Webbook
tb	484.20	K	NIST Webbook
tb	484.15 ± 2.00	K	NIST Webbook
tb	487.65 ± 1.00	K	NIST Webbook
tb	483.15 ± 2.00	K	NIST Webbook
tc	671.80 ± 0.50	K	NIST Webbook
tf	279.82	K	Aqueous Solubility Prediction Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.54	J/mol×K	568.46	Joback Method
cpg	420.12	J/mol×K	654.85	Joback Method
cpg	408.46	J/mol×K	626.06	Joback Method
cpg	396.27	J/mol×K	597.26	Joback Method
cpg	342.00	J/mol×K	482.07	Joback Method
cpg	356.42	J/mol×K	510.87	Joback Method
cpg	370.27	J/mol×K	539.66	Joback Method
dvisc	0.0002683	Pa×s	482.07	Joback Method
dvisc	0.0007090	Pa×s	367.23	Joback Method
dvisc	0.0004824	Pa×s	405.51	Joback Method
dvisc	0.0003508	Pa×s	443.79	Joback Method
dvisc	0.0045381	Pa×s	252.39	Joback Method
dvisc	0.0020766	Pa×s	290.67	Joback Method
dvisc	0.0011399	Pa×s	328.95	Joback Method
hvapt	44.60	kJ/mol	463.00	NIST Webbook
hvapt	55.10	kJ/mol	458.50	NIST Webbook
hvapt	51.70	kJ/mol	400.50	NIST Webbook
rhoI	820.63	kg/m ³	298.15	Excess molar enthalpies of binary mixtures containing 2-decanone or dipentyl ether with long-chain n-alkanes at T = 298.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49652e+01
Coeff. B	-4.23681e+03
Coeff. C	-7.55210e+01
Temperature range (K), min.	364.18
Temperature range (K), max.	514.40

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693549&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
Excess molar enthalpies of binary mixtures containing 2-decanone or diphenyl ether with long-chain n-alkanes at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.11.004
Aqueous Solubility Prediction Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
rhof:	Liquid 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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