3-Octanone, 2-methyl-

Other names:	2-Methyl-3-octanone
	2-methyloctan-3-one
	Isopropyl pentyl ketone
Inchi:	InChI=1S/C9H18O/c1-4-5-6-7-9(10)8(2)3/h8H,4-7H2,1-3H3
InchiKey:	ODSKXCNVESXQCZ-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCCCC(=O)C(C)C
Mol. weight [g/mol]:	142.24
CAS:	923-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-106.46	kJ/mol	Joback Method
hf	-346.95	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	41.99	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	984.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	984.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1322.00		NIST Webbook
tb	456.00 ± 4.00	K	NIST Webbook
tc	636.64	K	Joback Method
tf	226.12	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.82	J/mol×K	458.75	Joback Method
cpg	311.71	J/mol×K	488.40	Joback Method
cpg	325.02	J/mol×K	518.05	Joback Method
cpg	337.78	J/mol×K	547.69	Joback Method
cpg	350.00	J/mol×K	577.34	Joback Method
cpg	361.70	J/mol×K	606.99	Joback Method
cpg	372.87	J/mol×K	636.64	Joback Method
dvisc	0.0068479	Pa×s	226.12	Joback Method
dvisc	0.0026929	Pa×s	264.89	Joback Method
dvisc	0.0013439	Pa×s	303.66	Joback Method
dvisc	0.0007850	Pa×s	342.44	Joback Method
dvisc	0.0005116	Pa×s	381.21	Joback Method
dvisc	0.0003608	Pa×s	419.98	Joback Method
dvisc	0.0002699	Pa×s	458.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50693e+01
Coeff. B	-4.05583e+03
Coeff. C	-6.79180e+01
Temperature range (K), min.	342.30
Temperature range (K), max.	483.57

Sources

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=C923284&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume