3-Hexanone, 2-methyl-

Other names:	2-METHYL-3-HEXANONE
	2-Methylhexan-3-one
	Isopropyl propyl ketone
	Propyl isopropyl ketone
Inchi:	InChI=1S/C7H14O/c1-4-5-7(8)6(2)3/h6H,4-5H2,1-3H3
InchiKey:	HIGGFWFRAWSMBR-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCCC(=O)C(C)C
Mol. weight [g/mol]:	114.19
CAS:	7379-12-6

Physical Properties

Property code	Value	Unit	Source
gf	-123.30	kJ/mol	Joback Method
hf	-305.67	kJ/mol	Joback Method
hfus	11.96	kJ/mol	Joback Method
hvap	37.53	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	820.00		NIST Webbook
tb	412.99	K	Joback Method
tc	593.63	K	Joback Method
tf	203.58	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.88	J/mol×K	593.63	Joback Method
cpg	269.42	J/mol×K	563.52	Joback Method
cpg	259.52	J/mol×K	533.42	Joback Method
cpg	249.19	J/mol×K	503.31	Joback Method
cpg	238.41	J/mol×K	473.20	Joback Method
cpg	227.17	J/mol×K	443.10	Joback Method
cpg	215.47	J/mol×K	412.99	Joback Method
dvisc	0.0065747	Pa×s	203.58	Joback Method
dvisc	0.0002897	Pa×s	412.99	Joback Method
dvisc	0.0003833	Pa×s	378.09	Joback Method
dvisc	0.0005371	Pa×s	343.19	Joback Method
dvisc	0.0008121	Pa×s	308.28	Joback Method
dvisc	0.0013648	Pa×s	273.38	Joback Method
dvisc	0.0026700	Pa×s	238.48	Joback Method
hvapt	41.30	kJ/mol	351.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49031e+01
Coeff. B	-3.62991e+03
Coeff. C	-5.40600e+01
Temperature range (K), min.	302.42
Temperature range (K), max.	432.51

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1208.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7379126&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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