2-Hexanone, 4-methyl-

Other names: 4-Methyl-2-hexanone
4-Methylhexan-2-one
Methyl 2-methylbutyl ketone
Inchi: InChI=1S/C7H14O/c1-4-6(2)5-7(3)8/h6H,4-5H2,1-3H3
InchiKey: XUPXMIAWKPTZLZ-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CCC(C)CC(C)=O
Mol. weight [g/mol]: 114.19
CAS: 105-42-0

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	846.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		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	215.47	J/mol×K	412.99	Joback Method
cpg	227.17	J/mol×K	443.10	Joback Method

cpg	238.41	J/mol×K	473.20	Joback Method
cpg	249.19	J/mol×K	503.31	Joback Method
cpg	259.52	J/mol×K	533.42	Joback Method
cpg	269.42	J/mol×K	563.52	Joback Method
cpg	278.88	J/mol×K	593.63	Joback Method
dvisc	0.0065747	Pa×s	203.58	Joback Method
dvisc	0.0026700	Pa×s	238.48	Joback Method
dvisc	0.0013648	Pa×s	273.38	Joback Method
dvisc	0.0008121	Pa×s	308.28	Joback Method
dvisc	0.0005371	Pa×s	343.19	Joback Method
dvisc	0.0003833	Pa×s	378.09	Joback Method
dvisc	0.0002897	Pa×s	412.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49147e+01
Coeff. B	-3.67859e+03
Coeff. C	-5.57280e+01
Temperature range (K), min.	307.22
Temperature range (K), max.	438.79

Sources

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=C105420&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume