3-Hexen-2-one, 5-methyl-

Other names: 2-Oxo-5-methylhex-3-ene
3-Hexen-2-one, 5-Me
5-Methyl-3-hexen-2-one
5-methyl-hex-3-en-2-one
Inchi: InChI=1S/C7H12O/c1-6(2)4-5-7(3)8/h4-6H,1-3H3/b5-4+
InchiKey: IYMKNYVCXUEFJE-SNAWJCMRSA-N
Formula: C7H12O
SMILES: CC(=O)C=CC(C)C
Mol. weight [g/mol]: 112.17
CAS: 5166-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-43.08	kJ/mol	Joback Method
hf	-188.45	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	37.49	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.788		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	875.00		NIST Webbook
rinpol	912.00		NIST Webbook
ripol	1227.00		NIST Webbook
tb	417.15	K	Joback Method
tc	607.02	K	Joback Method
tf	198.50	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.13	J/mol×K	417.15	Joback Method
cpg	211.54	J/mol×K	448.80	Joback Method

cpg	222.38	J/mol×K	480.44	Joback Method
cpg	232.70	J/mol×K	512.09	Joback Method
cpg	242.50	J/mol×K	543.73	Joback Method
cpg	251.80	J/mol×K	575.38	Joback Method
cpg	260.64	J/mol×K	607.02	Joback Method
dvisc	0.0061552	Pa×s	198.50	Joback Method
dvisc	0.0023545	Pa×s	234.94	Joback Method
dvisc	0.0011658	Pa×s	271.38	Joback Method
dvisc	0.0006818	Pa×s	307.82	Joback Method
dvisc	0.0004467	Pa×s	344.27	Joback Method
dvisc	0.0003173	Pa×s	380.71	Joback Method
dvisc	0.0002393	Pa×s	417.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37838e+01
Coeff. B	-3.46752e+03
Coeff. C	-5.99520e+01
Temperature range (K), min.	316.88
Temperature range (K), max.	469.23

Sources

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=C5166530&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

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