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

Other names: 2-Methyl-1-hexene-5-one
5-Methyl-5-hexen-2-one
5-methylhex-5-en-2-one
Inchi: InChI=1S/C7H12O/c1-6(2)4-5-7(3)8/h1,4-5H2,2-3H3
InchiKey: VBCIOOKAKHGVMI-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=C(C)CCC(C)=O
Mol. weight [g/mol]: 112.17
CAS: 3240-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-41.57	kJ/mol	Joback Method
hf	-184.75	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	37.33	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	813.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	421.70	K	NIST Webbook
tb	422.00 ± 1.00	K	NIST Webbook
tc	593.82	K	Joback Method
tf	202.86	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	200.27	J/mol×K	409.99	Joback Method
cpg	211.18	J/mol×K	440.63	Joback Method
cpg	221.62	J/mol×K	471.27	Joback Method
cpg	231.59	J/mol×K	501.91	Joback Method
cpg	241.11	J/mol×K	532.54	Joback Method
cpg	250.19	J/mol×K	563.18	Joback Method
cpg	258.86	J/mol×K	593.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48160e+01
Coeff. B	-3.70089e+03
Coeff. C	-5.87860e+01
Temperature range (K), min.	313.52
Temperature range (K), max.	448.17

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3240093&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

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

Legend

cpg: Ideal gas heat capacity

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

ie:	Ionization energy
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