3-Penten-2-one, 3-methyl-

Other names: 3-Methyl-2-penten-4-one
3-Methyl-3-pentene-2-one
3-methyl-3-penten-2-one
3-methylpent-3-en-2-one
CH3CH=C(CH3)C(=O)CH3
Inchi: InChI=1S/C6H10O/c1-4-5(2)6(3)7/h4H,1-3H3/b5-4+
InchiKey: ZAMCMCQRTZKGDX-SNAWJCMRSA-N
Formula: C6H10O
SMILES: CC=C(C)C(C)=O
Mol. weight [g/mol]: 98.14
CAS: 565-62-8

Physical Properties

Property code	Value	Unit	Source
gf	-57.61	kJ/mol	Joback Method
hf	-172.32	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	35.73	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	859.00		NIST Webbook
rinpol	902.00		NIST Webbook
tb	411.20	K	NIST Webbook
tc	585.25	K	Joback Method
tf	188.27	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.72	J/mol×K	394.59	Joback Method

cpg	172.66	J/mol×K	426.37	Joback Method
cpg	182.11	J/mol×K	458.14	Joback Method
cpg	191.09	J/mol×K	489.92	Joback Method
cpg	199.62	J/mol×K	521.70	Joback Method
cpg	207.73	J/mol×K	553.47	Joback Method
cpg	215.42	J/mol×K	585.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.20	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46535e+01
Coeff. B	-3.56988e+03
Coeff. C	-5.54640e+01
Temperature range (K), min.	303.96
Temperature range (K), max.	437.59

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C565628&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume