3-Penten-2-one

Other names:	(E)-CH3CH=CHC(=O)CH3
	2-Oxo-3-pentene
	3-Pentene-2-one
	ETHYLIDENE ACETONE
	METHYL PROPENYL KETONE
	Methyl 1-propenyl ketone
	Pent-3-en-2-one
Inchi:	InChI=1S/C5H8O/c1-3-4-5(2)6/h3-4H,1-2H3
InchiKey:	LABTWGUMFABVFG-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CC=CC(C)=O
Mol. weight [g/mol]:	84.12
CAS:	625-33-2

Physical Properties

Property code	Value	Unit	Source
affp	864.30	kJ/mol	NIST Webbook
basg	832.50	kJ/mol	NIST Webbook
chl	-3041.00	kJ/mol	NIST Webbook
gf	-57.48	kJ/mol	Joback Method
hf	-136.00	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hvap	33.43	kJ/mol	Joback Method
ie	9.39	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	717.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	713.00		NIST Webbook

rinpol	731.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	714.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	709.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	719.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1121.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1112.00	NIST Webbook
ripol	1140.00	NIST Webbook
ripol	1137.00	NIST Webbook
ripol	1143.00	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1142.00	NIST Webbook
ripol	1128.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1139.00	NIST Webbook
ripol	1120.00	NIST Webbook
ripol	1120.00	NIST Webbook
ripol	1120.00	NIST Webbook
ripol	1132.00	NIST Webbook
ripol	1139.00	NIST Webbook

ripol	1147.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1119.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1119.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1138.00		NIST Webbook
tb	395.70	K	NIST Webbook
tc	559.72	K	Joback Method
tf	190.96	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.73	J/mol×K	371.83	Joback Method
cpg	136.10	J/mol×K	403.14	Joback Method
cpg	144.05	J/mol×K	434.46	Joback Method
cpg	151.61	J/mol×K	465.77	Joback Method
cpg	158.80	J/mol×K	497.09	Joback Method
cpg	165.62	J/mol×K	528.40	Joback Method
cpg	172.10	J/mol×K	559.72	Joback Method
dvisc	0.0030707	Pa×s	190.96	Joback Method
dvisc	0.0014998	Pa×s	221.11	Joback Method
dvisc	0.0008700	Pa×s	251.25	Joback Method
dvisc	0.0005671	Pa×s	281.39	Joback Method

dvisc	0.0004016	Pa×s	311.54	Joback Method
dvisc	0.0003022	Pa×s	341.68	Joback Method
dvisc	0.0002382	Pa×s	371.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46108e+01
Coeff. B	-3.44301e+03
Coeff. C	-5.11410e+01
Temperature range (K), min.	291.52
Temperature range (K), max.	421.38

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1221

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625332&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

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

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
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