1-Penten-3-one

Other names:	1-Pentene-3-one
	1-penten-3-one (ethyl vinyl ketone)
	C2H5COCH=CH2
	Ethyl vinyl ketone
	Ketone, ethyl vinyl
	Pent-1-en-3-one
	Vinyl ethyl ketone
	penten-3-one
Inchi:	InChI=1S/C5H8O/c1-3-5(6)4-2/h3H,1,4H2,2H3
InchiKey:	JLIDVCMBCGBIEY-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C=CC(=O)CC
Mol. weight [g/mol]:	84.12
CAS:	1629-58-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.86	kJ/mol	Joback Method
hf	-133.68	kJ/mol	Joback Method
hfpi	774.00	kJ/mol	NIST Webbook
hfus	9.03	kJ/mol	Joback Method
hvap	32.80	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	683.00		NIST Webbook

rinpol	683.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	684.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	654.00	NIST Webbook
rinpol	654.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	658.00	NIST Webbook
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rinpol	650.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	650.00	NIST Webbook
rinpol	676.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1020.00	NIST Webbook
ripol	1060.00	NIST Webbook
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ripol	1000.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1025.00	NIST Webbook

ripol	1025.00	NIST Webbook
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ripol	1023.00	NIST Webbook
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ripol	1018.00	NIST Webbook
ripol	973.00	NIST Webbook
ripol	1031.00	NIST Webbook
ripol	1036.00	NIST Webbook
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ripol	1009.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	973.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1022.00		NIST Webbook
tb	364.35	K	Joback Method
tc	546.41	K	Joback Method
tf	194.28	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.00	J/mol×K	546.41	Joback Method
cpg	165.61	J/mol×K	516.07	Joback Method
cpg	158.92	J/mol×K	485.72	Joback Method
cpg	151.91	J/mol×K	455.38	Joback Method
cpg	144.58	J/mol×K	425.04	Joback Method
cpg	136.92	J/mol×K	394.69	Joback Method
cpg	128.91	J/mol×K	364.35	Joback Method
dvisc	0.0028348	Pa×s	194.28	Joback Method
dvisc	0.0002808	Pa×s	364.35	Joback Method
dvisc	0.0003509	Pa×s	336.00	Joback Method
dvisc	0.0004569	Pa×s	307.66	Joback Method
dvisc	0.0006276	Pa×s	279.31	Joback Method
dvisc	0.0009261	Pa×s	250.97	Joback Method
dvisc	0.0015089	Pa×s	222.62	Joback Method
hvapt	36.70	kJ/mol	339.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	311.20	K	8.00	NIST Webbook
tbrp	375.20	K	98.70	NIST Webbook
tbrp	317.20	K	12.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39650e+01
Coeff. B	-3.14854e+03
Coeff. C	-4.57200e+01
Temperature range (K), min.	275.92
Temperature range (K), max.	409.56

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=C1629589&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

hfpi: Enthalpy of formation of positive ion at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume