3-Penten-2-one, (E)-

Other names:	(E)-3-Penten-2-one
	(E)-CH3C(O)CH=CHCH3
	trans-3-Penten-2-One
Inchi:	InChI=1S/C5H8O/c1-3-4-5(2)6/h3-4H,1-2H3/b4-3+
InchiKey:	LABTWGUMFABVFG-ONEGZZNKSA-N
Formula:	C5H8O
SMILES:	CC=CC(C)=O
Mol. weight [g/mol]:	84.12
CAS:	3102-33-8

Physical Properties

Property code	Value	Unit	Source
gf	-57.48	kJ/mol	Joback Method
hf	-141.89	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	33.43	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	714.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	712.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1104.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1122.00		NIST Webbook
ripol	1121.00		NIST Webbook

ripol	1108.00		NIST Webbook
tb	371.83	K	Joback Method
tc	559.72	K	Joback Method
tf	218.60 ± 0.60	K	NIST Webbook
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	1.59879e+01
Coeff. B	-3.76994e+03
Coeff. C	-5.10020e+01
Temperature range (K), min.	291.12
Temperature range (K), max.	404.11

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3102338&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
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