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

Other names:	2-methyl-1-penten-3-one
	Isopropenyl ethyl ketone
Inchi:	InChI=1S/C6H10O/c1-4-6(7)5(2)3/h2,4H2,1,3H3
InchiKey:	GHHGVSCQWPVENX-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C=C(C)C(=O)CC
Mol. weight [g/mol]:	98.14
CAS:	25044-01-3

Physical Properties

Property code	Value	Unit	Source
gf	-49.99	kJ/mol	Joback Method
hf	-164.11	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	35.11	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1068.00		NIST Webbook
tb	387.11	K	Joback Method
tc	572.11	K	Joback Method
tf	191.59	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/mol×K	387.11	Joback Method
cpg	172.98	J/mol×K	417.94	Joback Method
cpg	182.16	J/mol×K	448.78	Joback Method
cpg	190.92	J/mol×K	479.61	Joback Method
cpg	199.29	J/mol×K	510.45	Joback Method
cpg	207.28	J/mol×K	541.28	Joback Method
cpg	214.90	J/mol×K	572.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29739e+01
Coeff. B	-3.02304e+03
Coeff. C	-5.00290e+01
Temperature range (K), min.	288.32
Temperature range (K), max.	444.56

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=C25044013&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

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