1-Penten-3-one, 4-methyl-

Other names: Isopropyl vinyl ketone
iso-C3H7COCH=CH2
4-Methyl-1-penten-3-one
Inchi: InChI=1S/C6H10O/c1-4-6(7)5(2)3/h4-5H,1H2,2-3H3
InchiKey: SNOYUTZWILESAI-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C=CC(=O)C(C)C
Mol. weight [g/mol]: 98.14
CAS: 1606-47-9

Physical Properties

Property code	Value	Unit	Source
gf	-43.88	kJ/mol	Joback Method
hf	-159.60	kJ/mol	Joback Method
hfus	8.09	kJ/mol	Joback Method
hvap	34.64	kJ/mol	Joback Method
ie	9.39	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	1.397		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook
ripol	1093.00		NIST Webbook
ripol	1093.00		NIST Webbook
tb	386.79	K	Joback Method
tc	572.47	K	Joback Method
tf	190.55	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.35	J/mol×K	386.79	Joback Method

cpg	173.11	J/mol×K	417.74	Joback Method
cpg	182.44	J/mol×K	448.68	Joback Method
cpg	191.35	J/mol×K	479.63	Joback Method
cpg	199.86	J/mol×K	510.57	Joback Method
cpg	207.97	J/mol×K	541.52	Joback Method
cpg	215.70	J/mol×K	572.47	Joback Method
dvisc	0.0052215	Pa×s	190.55	Joback Method
dvisc	0.0022513	Pa×s	223.26	Joback Method
dvisc	0.0012035	Pa×s	255.96	Joback Method
dvisc	0.0007415	Pa×s	288.67	Joback Method
dvisc	0.0005041	Pa×s	321.38	Joback Method
dvisc	0.0003681	Pa×s	354.08	Joback Method
dvisc	0.0002834	Pa×s	386.79	Joback Method

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=C1606479&Units=SI
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
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
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