3-Penten-2-one, 3,4-dimethyl-

Other names: 3,4-Dimethyl-3-pentene-2-one
3,4-Dimethyl-3-penten-2-one
Inchi: InChI=1S/C7H12O/c1-5(2)6(3)7(4)8/h1-4H3
InchiKey: IZHBYIAZXCYIMS-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC(=O)C(C)=C(C)C
Mol. weight [g/mol]: 112.17
CAS: 684-94-6

Physical Properties

Property code	Value	Unit	Source
gf	-57.74	kJ/mol	Joback Method
hf	-202.75	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	38.04	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	914.00		NIST Webbook
tb	417.35	K	Joback Method
tc	610.34	K	Joback Method
tf	185.58	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.02	J/mol×K	417.35	Joback Method
cpg	211.45	J/mol×K	449.51	Joback Method
cpg	222.30	J/mol×K	481.68	Joback Method
cpg	232.62	J/mol×K	513.84	Joback Method
cpg	242.41	J/mol×K	546.01	Joback Method
cpg	251.71	J/mol×K	578.17	Joback Method

cpg	260.54	J/mol×K	610.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C684946&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume