3-Hexen-2-one, 3,4-dimethyl-

Other names: 3,4-Dimethyl-3-hexen-2-one
3,4-dimethylhex-3-en-2-one
Inchi: InChI=1S/C8H14O/c1-5-6(2)7(3)8(4)9/h5H2,1-4H3/b7-6+
InchiKey: WRHRFVOAEDXVPC-VOTSOKGWSA-N
Formula: C8H14O
SMILES: CCC(C)=C(C)C(C)=O
Mol. weight [g/mol]: 126.20
CAS: 1635-02-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.32	kJ/mol	Joback Method
hf	-223.39	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	440.23	K	Joback Method
tc	631.40	K	Joback Method
tf	196.85	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.59	J/mol×K	440.23	Joback Method
cpg	252.19	J/mol×K	472.09	Joback Method
cpg	264.18	J/mol×K	503.95	Joback Method
cpg	275.57	J/mol×K	535.81	Joback Method
cpg	286.40	J/mol×K	567.68	Joback Method
cpg	296.69	J/mol×K	599.54	Joback Method
cpg	306.46	J/mol×K	631.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25428e+01
Coeff. B	-3.17939e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	320.72
Temperature range (K), max.	500.96

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1635025&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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