4-Hexen-3-one, 4,5-dimethyl-

Other names: 4,5-dimethyl-4-hexen-3-one
Inchi: InChI=1S/C8H14O/c1-5-8(9)7(4)6(2)3/h5H2,1-4H3
InchiKey: CDMNXIBTIAFPBU-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CCC(=O)C(C)=C(C)C
Mol. weight [g/mol]: 126.20
CAS: 17325-90-5

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
rinpol	972.00		NIST Webbook
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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17325905&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