4-Hepten-3-one, 5-hydroxy-2,6-dimethyl-

Inchi: InChI=1S/C9H16O2/c1-6(2)8(10)5-9(11)7(3)4/h5-7,10H,1-4H3/b8-5-
InchiKey: JIYKPNNTWHWONK-YVMONPNESA-N
Formula: C9H16O2
SMILES: CC(C)C(=O)C=C(O)C(C)C
Mol. weight [g/mol]: 156.22
CAS: 34136-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-174.05	kJ/mol	Joback Method
hf	-397.03	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.309		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	554.53	K	Joback Method
tc	738.43	K	Joback Method
tf	252.90	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.73	J/mol×K	554.53	Joback Method
cpg	348.62	J/mol×K	585.18	Joback Method
cpg	359.92	J/mol×K	615.83	Joback Method
cpg	370.66	J/mol×K	646.48	Joback Method
cpg	380.85	J/mol×K	677.13	Joback Method
cpg	390.52	J/mol×K	707.78	Joback Method
cpg	399.70	J/mol×K	738.43	Joback Method

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=C34136022&Units=SI

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