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

Other names:	4,6-Dimethyl-5-hepten-2-one
	4,6-Dimethylhept-5-en-2-one
Inchi:	InChI=1S/C9H16O/c1-7(2)5-8(3)6-9(4)10/h5,8H,6H2,1-4H3
InchiKey:	SUBNDNOQXVTHOF-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CC(=O)CC(C)C=C(C)C
Mol. weight [g/mol]:	140.22
CAS:	31162-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-34.79	kJ/mol	Joback Method
hf	-239.52	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	42.02	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
ripol	1362.00		NIST Webbook
tb	462.79	K	Joback Method
tc	652.65	K	Joback Method
tf	207.08	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.53	J/mol×K	462.79	Joback Method
cpg	295.34	J/mol×K	494.43	Joback Method
cpg	308.48	J/mol×K	526.08	Joback Method
cpg	320.97	J/mol×K	557.72	Joback Method

cpg	332.84	J/mol×K	589.36	Joback Method
cpg	344.12	J/mol×K	621.01	Joback Method
cpg	354.83	J/mol×K	652.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31162488&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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