2-Cyclopenten-1-one, 4-acetyl-2,3,4,5,5-pentamethyl-

Other names: 2-Cyclopenten-1-one, 4-acetyl-1,2,3,5,5-pentamethyl
Inchi: InChI=1S/C12H18O2/c1-7-8(2)12(6,9(3)13)11(4,5)10(7)14/h1-6H3
InchiKey: XPYNAEMDBLPZGA-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(=O)C1(C)C(C)=C(C)C(=O)C1(C)C
Mol. weight [g/mol]: 194.27
CAS: 50506-59-7

Physical Properties

Property code	Value	Unit	Source
gf	-172.79	kJ/mol	Joback Method
hf	-435.83	kJ/mol	Joback Method
hfus	10.80	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.527		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
tb	615.86	K	Joback Method
tc	843.56	K	Joback Method
tf	423.41	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.64	J/mol×K	615.86	Joback Method
cpg	452.95	J/mol×K	653.81	Joback Method
cpg	468.59	J/mol×K	691.76	Joback Method
cpg	483.73	J/mol×K	729.71	Joback Method
cpg	498.57	J/mol×K	767.66	Joback Method
cpg	513.29	J/mol×K	805.61	Joback Method
cpg	528.08	J/mol×K	843.56	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=C50506597&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