2-Isopropenyl-5-methyl-4-oxo-hex-5-enyl acetate

Inchi: InChI=1S/C12H18O3/c1-8(2)11(7-15-10(5)13)6-12(14)9(3)4/h11H,1,3,6-7H2,2,4-5H3
InchiKey: YIMBTHHLSRBHFF-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: C=C(C)C(=O)CC(COC(C)=O)C(=C)C
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-156.54	kJ/mol	Joback Method
hf	-422.39	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.277		Crippen Method
mcvol	180.350	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1388.00		NIST Webbook
ripol	1991.00		NIST Webbook
tb	596.80	K	Joback Method
tc	789.73	K	Joback Method
tf	300.65	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.47	J/mol×K	596.80	Joback Method
cpg	460.76	J/mol×K	628.96	Joback Method
cpg	474.33	J/mol×K	661.11	Joback Method
cpg	487.18	J/mol×K	693.27	Joback Method
cpg	499.35	J/mol×K	725.42	Joback Method
cpg	510.85	J/mol×K	757.58	Joback Method
cpg	521.69	J/mol×K	789.73	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=R232401&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
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