2,6-Dimethyl-1,7-octadien-3-ol, acetate

Other names: 1-isopropenyl-4-methylhex-5-enyl acetate
Inchi: InChI=1S/C12H20O2/c1-6-10(4)7-8-12(9(2)3)14-11(5)13/h6,10,12H,1-2,7-8H2,3-5H3
InchiKey: ATOCHKMVAHBPNF-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=CC(C)CCC(OC(C)=O)C(=C)C
Mol. weight [g/mol]: 196.29
CAS: 61382-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-21.51	kJ/mol	Joback Method
hf	-305.30	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	49.43	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.096		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
tb	542.61	K	Joback Method
tc	728.14	K	Joback Method
tf	249.68	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.09	J/mol×K	542.61	Joback Method
cpg	440.64	J/mol×K	573.53	Joback Method
cpg	455.47	J/mol×K	604.45	Joback Method
cpg	469.60	J/mol×K	635.38	Joback Method
cpg	483.04	J/mol×K	666.30	Joback Method
cpg	495.83	J/mol×K	697.22	Joback Method
cpg	507.97	J/mol×K	728.14	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=C61382998&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