Ho-trienyl acetate

Other names: Ho-trienol, acetate
Inchi: InChI=1S/C12H18O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6-8H,1-2,9H2,3-5H3/b8-7+
InchiKey: BTTUBYGGUJLPGO-BQYQJAHWSA-N
Formula: C12H18O2
SMILES: C=CC(C)(CC=CC(=C)C)OC(C)=O
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	66.43	kJ/mol	Joback Method
hf	-186.27	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.017		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
tb	544.42	K	Joback Method
tc	741.16	K	Joback Method
tf	277.02	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.23	J/mol×K	544.42	Joback Method
cpg	424.60	J/mol×K	577.21	Joback Method
cpg	439.08	J/mol×K	610.00	Joback Method
cpg	452.71	J/mol×K	642.79	Joback Method
cpg	465.54	J/mol×K	675.58	Joback Method
cpg	477.62	J/mol×K	708.37	Joback Method

cpg	489.00	J/mol×K	741.16	Joback Method

Sources

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=R130013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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