2,6-Dimethyl-1,6-heptadien-4-ol acetate

Inchi: InChI=1S/C11H18O2/c1-8(2)6-11(7-9(3)4)13-10(5)12/h11H,1,3,6-7H2,2,4-5H3
InchiKey: NAASNCRONHZOQA-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=C(C)CC(CC(=C)C)OC(C)=O
Mol. weight [g/mol]: 182.26
CAS: 70187-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-36.04	kJ/mol	Joback Method
hf	-289.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	47.67	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.850		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
tb	520.05	K	Joback Method
tc	707.10	K	Joback Method
tf	239.45	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.26	J/mol×K	520.05	Joback Method
cpg	391.92	J/mol×K	551.23	Joback Method
cpg	405.90	J/mol×K	582.40	Joback Method
cpg	419.24	J/mol×K	613.58	Joback Method
cpg	431.94	J/mol×K	644.75	Joback Method
cpg	444.03	J/mol×K	675.93	Joback Method
cpg	455.51	J/mol×K	707.10	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=C70187916&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume