(Z)-3,7-Dimethyl-2,7-octadien-1-ol, propanoate(ester)

Inchi: InChI=1S/C13H22O2/c1-5-13(14)15-10-9-12(4)8-6-7-11(2)3/h9H,2,5-8,10H2,1,3-4H3/b12
InchiKey: NACFFFPZCNALMT-XFXZXTDPSA-N
Formula: C13H22O2
SMILES: C=C(C)CCCC(C)=CCOC(=O)CC
Mol. weight [g/mol]: 210.31
CAS: 73214-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.38	kJ/mol	Joback Method
hf	-333.38	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1422.00		NIST Webbook
tb	573.73	K	Joback Method
tc	757.29	K	Joback Method
tf	273.67	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.77	J/mol×K	573.73	Joback Method
cpg	490.63	J/mol×K	604.32	Joback Method
cpg	505.74	J/mol×K	634.92	Joback Method
cpg	520.13	J/mol×K	665.51	Joback Method
cpg	533.83	J/mol×K	696.10	Joback Method
cpg	546.87	J/mol×K	726.70	Joback Method
cpg	559.27	J/mol×K	757.29	Joback Method

Sources

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=C73214627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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