7-Methyl-3-methylene-7-octen-1-ol, propanoate (ester)

Inchi: InChI=1S/C13H22O2/c1-5-13(14)15-10-9-12(4)8-6-7-11(2)3/h2,4-10H2,1,3H3
InchiKey: KRONWWNTASLWRC-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=C(C)CCCC(=C)CCOC(=O)CC
Mol. weight [g/mol]: 210.31
CAS: 73214-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-16.76	kJ/mol	Joback Method
hf	-325.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	1415.00		NIST Webbook
tb	566.25	K	Joback Method
tc	745.89	K	Joback Method
tf	276.99	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.39	J/mol×K	566.25	Joback Method
cpg	489.11	J/mol×K	596.19	Joback Method
cpg	504.12	J/mol×K	626.13	Joback Method
cpg	518.44	J/mol×K	656.07	Joback Method
cpg	532.10	J/mol×K	686.01	Joback Method
cpg	545.11	J/mol×K	715.95	Joback Method
cpg	557.50	J/mol×K	745.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73214638&Units=SI
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

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