methyl dihydroepijasmonate

Inchi: InChI=1S/C13H22O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h10-11H,3-9H2,1-2H3
InchiKey: KVWWIYGFBYDJQC-MNOVXSKESA-N
Formula: C13H22O3
SMILES: CCCCCC1C(=O)CCC1CC(=O)OC
Mol. weight [g/mol]: 226.31
CAS: 39647-11-5

Physical Properties

Property code	Value	Unit	Source
gf	-269.09	kJ/mol	Joback Method
hf	-654.01	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	57.88	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.725		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1649.00		NIST Webbook
tb	651.56	K	Joback Method
tc	854.07	K	Joback Method
tf	383.31	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.32	J/mol×K	651.56	Joback Method
cpg	562.70	J/mol×K	685.31	Joback Method
cpg	580.11	J/mol×K	719.06	Joback Method
cpg	596.55	J/mol×K	752.81	Joback Method
cpg	612.00	J/mol×K	786.57	Joback Method
cpg	626.46	J/mol×K	820.32	Joback Method
cpg	639.93	J/mol×K	854.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39647115&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