Methyl (Z)-dihydrojasmonate

Other names: cis-Methyl dihydrojasmonate
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-QWRGUYRKSA-N
Formula: C13H22O3
SMILES: CCCCCC1C(=O)CCC1CC(=O)OC
Mol. weight [g/mol]: 226.31

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	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1656.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		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

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=R417746&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume