(Z)-Methyl epi-jasmonate

Inchi: InChI=1S/C12H18O3/c1-3-4-5-6-9-10(12(14)15-2)7-8-11(9)13/h4-5,9-10H,3,6-8H2,1-2H3
InchiKey: LQBORWCRYHAYHJ-NDVXOHMPSA-N
Formula: C12H18O3
SMILES: CCC=CCC1C(=O)CCC1C(=O)OC
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-197.29	kJ/mol	Joback Method
hf	-516.15	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	55.61	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.111		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	632.84	K	Joback Method
tc	846.51	K	Joback Method
tf	366.96	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.19	J/mol×K	632.84	Joback Method
cpg	487.70	J/mol×K	668.45	Joback Method
cpg	504.24	J/mol×K	704.06	Joback Method
cpg	519.80	J/mol×K	739.68	Joback Method
cpg	534.40	J/mol×K	775.29	Joback Method
cpg	548.03	J/mol×K	810.90	Joback Method
cpg	560.71	J/mol×K	846.51	Joback Method

Sources

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=R285995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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