(Z)-methyl 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-YVDHIRPGSA-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	1649.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1647.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2404.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2407.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R286007&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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