(+)-Jasmonic acid, methyl ester (cis)

Inchi: InChI=1S/C13H20O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h4-5,10-11H,3,6-9H2,
InchiKey: GEWDNTWNSAZUDX-NRFYAWERSA-N
Formula: C13H20O3
SMILES: CCC=CCC1C(=O)CCC1CC(=O)OC
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	-188.87	kJ/mol	Joback Method
hf	-536.79	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	57.84	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.501		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	655.72	K	Joback Method
tc	866.01	K	Joback Method
tf	378.23	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.90	J/mol×K	655.72	Joback Method
cpg	540.85	J/mol×K	690.77	Joback Method
cpg	557.79	J/mol×K	725.82	Joback Method
cpg	573.72	J/mol×K	760.87	Joback Method
cpg	588.65	J/mol×K	795.91	Joback Method
cpg	602.59	J/mol×K	830.96	Joback Method
cpg	615.53	J/mol×K	866.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R169576&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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