Methyl jasmonate

Other names:	Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester, [1R-[1«alpha»,2«beta»(Z)]]- Cyclopentaneacetic acid, 3-oxo-2-(2Z)-2-penten-1-yl-, methyl ester, (1R,2R)- Cyclopentaneacetic acid, 3-oxo-trans-2-(cis-2-pentenyl), methyl ester Z-Methyl jasmonoate Methyl cis-jasmonate methyl [1R-[1«alpha»,2«beta»(Z)]]-3-oxo-2-(pent-2-enyl)cyclopentaneacetate
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-NNOMMRTBSA-N
Formula:	C13H20O3
SMILES:	CCC=CCC1C(=O)CCC1CC(=O)OC
Mol. weight [g/mol]:	224.30
CAS:	1211-29-6

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	1612.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1655.40		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1655.40		NIST Webbook
rinpol	1652.00		NIST Webbook

ripol	2338.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2345.00		NIST Webbook
ripol	2332.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1211296&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume