

# (-)-Jasmonic acid, methyl ester (trans)

<b>Inchi:</b>	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
<b>InchiKey:</b>	GEWDNTWNSAZUDX-XXJOZFEBSA-N
<b>Formula:</b>	C13H20O3
<b>SMILES:</b>	CCC=CCC1C(=O)CCC1CC(=O)OC
<b>Mol. weight [g/mol]:</b>	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
rinqol	1605.00		NIST Webbook
tb	655.72	K	Joback Method
tc	866.01	K	Joback Method
tf	378.23	K	Joback Method
vc	0.715	m <sup>3</sup> /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

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R169605&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R169605&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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