

# (+)-Jasmonic acid - (S)-Val conjugate, methyl ester

Inchi:	InChI=1S/C18H29NO4/c1-5-6-7-8-14-13(9-10-15(14)20)11-16(21)19-17(12(2)3)18(22)23
InchiKey:	GDPPAUUXPQZOBY-JKVOCJEQSA-N
Formula:	C18H29NO4
SMILES:	CCC=CCC1C(=O)CCC1CC(=O)NC(C(=O)OC)C(C)C
Mol. weight [g/mol]:	323.43

## Physical Properties

Property code	Value	Unit	Source
gf	-191.18	kJ/mol	Joback Method
hf	-709.66	kJ/mol	Joback Method
hfus	39.53	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.642		Crippen Method
mcvol	269.880	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinsol	2291.00		NIST Webbook
tb	873.28	K	Joback Method
tc	1086.95	K	Joback Method
tf	507.17	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.39	J/mol×K	873.28	Joback Method
cpg	904.91	J/mol×K	908.89	Joback Method
cpg	920.05	J/mol×K	944.50	Joback Method
cpg	933.85	J/mol×K	980.12	Joback Method
cpg	946.32	J/mol×K	1015.73	Joback Method
cpg	957.48	J/mol×K	1051.34	Joback Method
cpg	967.37	J/mol×K	1086.95	Joback Method

# Sources

<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=R169596&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R169596&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>hvap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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