

# Methyl 13«beta»-Abieta-7,9(11)dien-18-oate

<b>Inchi:</b>	InChI=1S/C21H32O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2)
<b>InchiKey:</b>	HALJWOPQKXPVQL-HGWQEYRNSA-N
<b>Formula:</b>	C21H32O2
<b>SMILES:</b>	COC(=O)C1(C)CCCC2(C)C3=CCC(C(C)C)CC3=CCC12
<b>Mol. weight [g/mol]:</b>	316.48

## Physical Properties

Property code	Value	Unit	Source
gf	33.30	kJ/mol	Joback Method
hf	-436.49	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.295		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2278.00		NIST Webbook
tb	801.39	K	Joback Method
tc	1033.26	K	Joback Method
tf	489.93	K	Joback Method
vc	1.028	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.67	J/molxK	801.39	Joback Method
cpg	911.14	J/molxK	840.03	Joback Method
cpg	935.22	J/molxK	878.68	Joback Method
cpg	959.20	J/molxK	917.32	Joback Method
cpg	983.38	J/molxK	955.97	Joback Method
cpg	1008.04	J/molxK	994.61	Joback Method
cpg	1033.50	J/molxK	1033.26	Joback Method

# Sources

<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>
<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=R20366&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R20366&amp;Units=SI</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>h vap:</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>m cvol:</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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