

# trans-«alpha»-bergamatol acetate

<b>Inchi:</b>	InChI=1S/C17H26O2/c1-12(11-19-14(3)18)6-5-9-17(4)15-8-7-13(2)16(17)10-15/h6-7,15-
<b>InchiKey:</b>	BDYQEBZJCFGMCH-VHBUNTFRSA-N
<b>Formula:</b>	C17H26O2
<b>SMILES:</b>	CC(=O)OCC(C)=CCCC1(C)C2CC=C(C)C1C2
<b>Mol. weight [g/mol]:</b>	262.39

## Physical Properties

Property code	Value	Unit	Source
gf	46.54	kJ/mol	Joback Method
hf	-350.93	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinsol	1801.00		NIST Webbook
tb	686.15	K	Joback Method
tc	892.39	K	Joback Method
tf	399.77	K	Joback Method
vc	0.881	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.76	J/mol×K	686.15	Joback Method
cpg	678.74	J/mol×K	720.52	Joback Method
cpg	696.87	J/mol×K	754.90	Joback Method
cpg	714.28	J/mol×K	789.27	Joback Method
cpg	731.12	J/mol×K	823.64	Joback Method
cpg	747.53	J/mol×K	858.02	Joback Method
cpg	763.66	J/mol×K	892.39	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=R238350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R238350&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>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>mccvol:</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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