

# trans-Verbenyl acetate

<b>Inchi:</b>	InChI=1S/C12H18O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h5,9-11H,6H2,1-4H3/t9-,1
<b>InchiKey:</b>	OZBFUQLOVFXDNK-HBNTYKKESA-N
<b>Formula:</b>	C12H18O2
<b>SMILES:</b>	CC(=O)OC1C=C(C)C2CC1C2(C)C
<b>Mol. weight [g/mol]:</b>	194.27

## Physical Properties

Property code	Value	Unit	Source
gf	-74.94	kJ/mol	Joback Method
hf	-375.50	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	563.04	K	Joback Method
tc	773.40	K	Joback Method
tf	358.22	K	Joback Method
vc	0.620	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.92	J/mol×K	563.04	Joback Method
cpg	437.32	J/mol×K	598.10	Joback Method
cpg	453.71	J/mol×K	633.16	Joback Method
cpg	469.20	J/mol×K	668.22	Joback Method
cpg	483.90	J/mol×K	703.28	Joback Method
cpg	497.94	J/mol×K	738.34	Joback Method
cpg	511.43	J/mol×K	773.40	Joback Method

# Sources

<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=R626910&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R626910&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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