

# trans-Sabinene hydrate acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-8(2)12-6-5-11(4,10(12)7-12)14-9(3)13/h8,10H,5-7H2,1-4H3/t10
<b>InchiKey:</b>	MYCFGFMJUUNKBN-RAMGSTBQSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	CC(=O)OC1(C)CCC2(C(C)C)CC12
<b>Mol. weight [g/mol]:</b>	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-83.39	kJ/mol	Joback Method
hf	-385.35	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	48.29	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1286.00		NIST Webbook
tb	559.10	K	Joback Method
tc	772.02	K	Joback Method
tf	361.60	K	Joback Method
vc	0.634	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.10	J/molxK	559.10	Joback Method
cpg	453.75	J/molxK	594.59	Joback Method
cpg	470.23	J/molxK	630.07	Joback Method
cpg	485.75	J/molxK	665.56	Joback Method
cpg	500.56	J/molxK	701.04	Joback Method
cpg	514.85	J/molxK	736.53	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=R607528&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R607528&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>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>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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