

# Thujyl acetate

Other names:3-Thujyl acetate

Inchi:InChI=1S/C12H20O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7-8,10-11H,5-6H2,1-4H

InchiKey:RYMWIDNPMDLHRP-UHFFFAOYSA-N

Formula:C12H20O2

SMILES:CC(=O)OC1CC2(C(C)C)CC2C1C

Mol. weight [g/mol]:196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-85.61	kJ/mol	Joback Method
hf	-420.93	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.620		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1290.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1542.00		NIST Webbook
tb	554.19	K	Joback Method
tc	758.84	K	Joback Method
tf	333.46	K	Joback Method
vc	0.635	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.10	J/molxK	554.19	Joback Method
cpg	456.42	J/molxK	588.30	Joback Method
cpg	473.65	J/molxK	622.41	Joback Method
cpg	489.90	J/molxK	656.52	Joback Method
cpg	505.31	J/molxK	690.62	Joback Method
cpg	519.99	J/molxK	724.73	Joback Method
cpg	534.06	J/molxK	758.84	Joback Method

## Sources

<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>
<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=R129810&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R129810&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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