

# «delta»-Terpineol, acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h11H,1,5-8H2,2-4H3
<b>InchiKey:</b>	IWKXKWUCSZHJEK-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	C=C1CCC(C(C)(C)OC(C)=O)CC1
<b>Mol. weight [g/mol]:</b>	196.29
<b>CAS:</b>	93836-50-1

## Physical Properties

Property code	Value	Unit	Source
gf	-103.39	kJ/mol	Joback Method
hf	-406.00	kJ/mol	Joback Method
hfus	12.88	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1316.10		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1316.10		NIST Webbook
tb	565.73	K	Joback Method
tc	778.96	K	Joback Method
tf	320.64	K	Joback Method
vc	0.637	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.96	J/molxK	565.73	Joback Method
cpg	456.01	J/molxK	601.27	Joback Method
cpg	473.94	J/molxK	636.81	Joback Method
cpg	490.78	J/molxK	672.34	Joback Method
cpg	506.57	J/molxK	707.88	Joback Method
cpg	521.33	J/molxK	743.42	Joback Method

cpg	535.11	J/mol×K	778.96	Joback Method
dvisc	0.0031095	Paxs	320.64	Joback Method
dvisc	0.0015253	Paxs	361.49	Joback Method
dvisc	0.0008647	Paxs	402.34	Joback Method
dvisc	0.0005442	Paxs	443.19	Joback Method
dvisc	0.0003704	Paxs	484.03	Joback Method
dvisc	0.0002676	Paxs	524.88	Joback Method
dvisc	0.0002027	Paxs	565.73	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C93836501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93836501&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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