

# Trematol (21-epi-9[11]-farnenol) acetate

<b>Inchi:</b>	InChI=1S/C32H52O2/c1-20(2)22-10-13-26-30(22,7)18-19-31(8)24-11-12-25-28(4,5)27(3)
<b>InchiKey:</b>	WQWTUUFHPFYTRZ-HLEDKMHISA-N
<b>Formula:</b>	C32H52O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C3=CCC4(C)C5CCC(C(C)C)C5(C)CCC4(C)C3CCC2C1(C)C
<b>Mol. weight [g/mol]:</b>	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	167.68	kJ/mol	Joback Method
hf	-606.04	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinsol	3489.00		NIST Webbook
tb	1048.72	K	Joback Method
tc	1296.76	K	Joback Method
tf	687.72	K	Joback Method
vc	1.554	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1688.55	J/mol×K	1048.72	Joback Method
cpg	1749.18	J/mol×K	1090.06	Joback Method
cpg	1815.48	J/mol×K	1131.40	Joback Method
cpg	1888.28	J/mol×K	1172.74	Joback Method
cpg	1968.41	J/mol×K	1214.08	Joback Method
cpg	2056.69	J/mol×K	1255.42	Joback Method
cpg	2153.95	J/mol×K	1296.76	Joback Method

# Sources

<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=R111483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111483&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>
<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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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