

# Tocotrienol, 5,7,8-trimethyl

<b>Inchi:</b>	InChI=1S/C29H44O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7)
<b>InchiKey:</b>	RZFHLOLGZPDCHJ-AIEICBQISA-N
<b>Formula:</b>	C29H44O2
<b>SMILES:</b>	CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2c(C)c(O)c(C)c(C)c2O1
<b>Mol. weight [g/mol]:</b>	424.66

## Physical Properties

Property code	Value	Unit	Source
gf	284.62	kJ/mol	Joback Method
hf	-356.38	kJ/mol	Joback Method
hfus	63.53	kJ/mol	Joback Method
hvap	101.64	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	8.601		Crippen Method
mcvol	383.690	ml/mol	McGowan Method
pc	964.47	kPa	Joback Method
rinpol	3208.00		NIST Webbook
tb	1040.46	K	Joback Method
tc	1276.15	K	Joback Method
tf	612.58	K	Joback Method
vc	1.429	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.13	J/molxK	1040.46	Joback Method
cpg	1383.27	J/molxK	1079.74	Joback Method
cpg	1414.60	J/molxK	1119.02	Joback Method
cpg	1447.46	J/molxK	1158.31	Joback Method
cpg	1482.18	J/molxK	1197.59	Joback Method
cpg	1519.07	J/molxK	1236.87	Joback Method
cpg	1558.48	J/molxK	1276.15	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=R523009&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523009&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>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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