

# Tocol, 5-methyl

**Inchi:** InChI=1S/C27H46O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-18-27(6)19-17-24-23(5)25  
**InchiKey:** CUZJBNKZWVQOPX-BERHBOFZSA-N  
**Formula:** C27H46O2  
**SMILES:** Cc1c(O)ccc2c1CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2  
**Mol. weight [g/mol]:** 402.65

## Physical Properties

Property code	Value	Unit	Source
gf	64.71	kJ/mol	Joback Method
hf	-630.29	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	94.59	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.223		Crippen Method
mvol	368.410	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	971.30	K	Joback Method
tc	1192.37	K	Joback Method
tf	577.12	K	Joback Method
vc	1.355	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.97	J/molxK	971.30	Joback Method
cpg	1325.79	J/molxK	1008.14	Joback Method
cpg	1351.73	J/molxK	1044.99	Joback Method
cpg	1378.03	J/molxK	1081.83	Joback Method
cpg	1404.92	J/molxK	1118.68	Joback Method
cpg	1432.64	J/molxK	1155.52	Joback Method
cpg	1461.41	J/molxK	1192.37	Joback Method

# Sources

<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=R522957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522957&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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