

# Tomatidine

**Other names:**

Spirosolan-3-ol, (3«beta»,5«alpha»,22«beta»,25S)-  
5«alpha»-Tomatidan-3«beta»-ol  
Tomatidin

**Inchi:** InChI=1S/C27H45NO2/c1-16-7-12-27(28-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19**InchiKey:** XYNPYHXGMWJBLV-PQEHJEBQSA-N**Formula:** C27H45NO2**SMILES:** CC1CCC2(NC1)OC1CC3C4CCC5CC(O)CCC5(C)C4CCC3(C)C1C2C**Mol. weight [g/mol]:** 415.65**CAS:** 77-59-8

## Physical Properties

Property code	Value	Unit	Source
gf	258.30	kJ/mol	Joback Method
hf	-529.67	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.367		Crippen Method
mcvol	347.850	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinsol	3370.00		NIST Webbook
tb	1027.87	K	Joback Method
tc	1273.00	K	Joback Method
tf	715.73	K	Joback Method
vc	1.298	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.39	J/mol×K	1027.87	Joback Method
cpg	1505.04	J/mol×K	1068.73	Joback Method
cpg	1550.34	J/mol×K	1109.58	Joback Method
cpg	1598.85	J/mol×K	1150.44	Joback Method
cpg	1651.15	J/mol×K	1191.29	Joback Method

cpg	1707.80	J/mol×K	1232.15	Joback Method
cpg	1769.37	J/mol×K	1273.00	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=C77598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C77598&amp;Units=SI</a>
<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.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>rinpolar:</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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