

# cis-Totarol

<b>Inchi:</b>	InChI=1S/C20H30O/c1-13(2)18-14-7-10-17-19(3,4)11-6-12-20(17,5)15(14)8-9-16(18)21/
<b>InchiKey:</b>	ZRVDANDJSTYELM-PXNSSMCTSA-N
<b>Formula:</b>	C20H30O
<b>SMILES:</b>	CC(C)c1c(O)ccc2c1CCC1C(C)(C)CCCC21C
<b>Mol. weight [g/mol]:</b>	286.45

## Physical Properties

Property code	Value	Unit	Source
gf	132.22	kJ/mol	Joback Method
hf	-281.71	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.546		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2276.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2257.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	791.65	K	Joback Method
tc	1034.71	K	Joback Method
tf	535.74	K	Joback Method
vc	0.900	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	807.54	J/mol×K	791.65	Joback Method
cpg	831.05	J/mol×K	832.16	Joback Method
cpg	854.62	J/mol×K	872.67	Joback Method
cpg	878.69	J/mol×K	913.18	Joback Method
cpg	903.66	J/mol×K	953.69	Joback Method
cpg	929.95	J/mol×K	994.20	Joback Method
cpg	957.98	J/mol×K	1034.71	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.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>
<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=R301938&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R301938&amp;Units=SI</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>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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