

# Gitogenin

<b>Inchi:</b>	InChI=1S/C27H44O4/c1-15-7-10-27(30-14-15)16(2)24-23(31-27)12-20-18-6-5-17-11-21(
<b>InchiKey:</b>	FWCXELAAAYFYCSR-UHFFFAOYSA-N
<b>Formula:</b>	C27H44O4
<b>SMILES:</b>	CC1CCC2(OC1)OC1CC3C4CCC5CC(O)C(O)CC5(C)C4CCC3(C)C1C2C
<b>Mol. weight [g/mol]:</b>	432.64
<b>CAS:</b>	6811-13-8

## Physical Properties

Property code	Value	Unit	Source
gf	-60.06	kJ/mol	Joback Method
hf	-872.05	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	113.14	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.765		Crippen Method
mcvol	349.610	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
tb	1093.78	K	Joback Method
tc	1340.02	K	Joback Method
tf	693.85	K	Joback Method
vc	1.300	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1545.31	J/molxK	1093.78	Joback Method
cpg	1592.37	J/molxK	1134.82	Joback Method
cpg	1643.02	J/molxK	1175.86	Joback Method
cpg	1697.83	J/molxK	1216.90	Joback Method
cpg	1757.40	J/molxK	1257.94	Joback Method
cpg	1822.30	J/molxK	1298.98	Joback Method
cpg	1893.10	J/molxK	1340.02	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=C6811138&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6811138&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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