

# C28 5A,14B,17B,20S-Sterane

**Inchi:** InChI=1S/C28H50/c1-19(2)20(3)10-11-21(4)24-14-15-25-23-13-12-22-9-7-8-17-27(22,5)  
**InchiKey:** WAAWMJYYKITCGF-JUCQXXNFSA-N  
**Formula:** C28H50  
**SMILES:** CC(C)C(C)CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 386.70

## Physical Properties

Property code	Value	Unit	Source
gf	325.95	kJ/mol	Joback Method
hf	-407.23	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	74.04	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.744		Crippen Method
mcvol	361.940	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	2917.00		NIST Webbook
tb	873.50	K	Joback Method
tc	1096.28	K	Joback Method
tf	449.56	K	Joback Method
vc	1.367	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.06	J/mol×K	873.50	Joback Method
cpg	1351.20	J/mol×K	910.63	Joback Method
cpg	1383.04	J/mol×K	947.76	Joback Method
cpg	1414.91	J/mol×K	984.89	Joback Method
cpg	1447.16	J/mol×K	1022.02	Joback Method
cpg	1480.10	J/mol×K	1059.15	Joback Method
cpg	1514.07	J/mol×K	1096.28	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=R56183&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R56183&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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