

Gorgost-5-en-3-ol, (3«beta»)-

Other names:	Pregn-5-en-3«beta»-ol, 20«alpha»-[(1R,2R)-2-(1R)-1,2-dimethylpropyl-2-methylcyclopropyl]- Gorgosterol
Inchi:	InChI=1S/C30H50O/c1-18(2)20(4)30(7)17-27(30)19(3)24-10-11-25-23-9-8-21-16-22(31)
InchiKey:	YRPMZHRSQIFCLR-HNDSVRFXSA-N
Formula:	C30H50O
SMILES:	CC(C)C(C)C1(C)CC1C(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	426.72
CAS:	29782-65-8

Physical Properties

Property code	Value	Unit	Source
gf	273.85	kJ/mol	Joback Method
hf	-486.73	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	94.58	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.881		Crippen Method
mcvol	380.830	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	3420.00		NIST Webbook
rinpol	3420.00		NIST Webbook
tb	1017.89	K	Joback Method
tc	1252.11	K	Joback Method
tf	583.80	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1527.72	J/molxK	1017.89	Joback Method
cpg	1569.62	J/molxK	1056.93	Joback Method
cpg	1614.02	J/molxK	1095.96	Joback Method
cpg	1661.44	J/molxK	1135.00	Joback Method
cpg	1712.41	J/molxK	1174.04	Joback Method

cpg	1767.44	J/mol×K	1213.08	Joback Method
cpg	1827.06	J/mol×K	1252.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29782658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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