5-«alpha»-Cholest-22-en-3-«beta»-ol, cis

Inchi: InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey: BWGQUGBECNWWDB-VSSCPYPWSA-N
Formula: C27H46O
SMILES: CC(C)CC=CC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 386.65

Physical Properties

Property code	Value	Unit	Source
gf	255.66	kJ/mol	Joback Method
hf	-436.66	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	7.245		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	942.73	K	Joback Method
tc	1165.42	K	Joback Method
tf	504.79	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1322.83	J/mol×K	942.73	Joback Method
cpg	1353.67	J/mol×K	979.84	Joback Method
cpg	1384.97	J/mol×K	1016.96	Joback Method
cpg	1417.07	J/mol×K	1054.07	Joback Method
cpg	1450.30	J/mol×K	1091.19	Joback Method
cpg	1485.00	J/mol×K	1128.30	Joback Method
cpg	1521.51	J/mol×K	1165.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215095&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume