5-«alpha»-Cholesta-7,22-dien-3-«beta»-ol

Inchi: InChI=1S/C27H44O/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: KJOAIBPHMYWAOX-ODMXCDLMSA-N
Formula: C27H44O
SMILES: CC(C)CC=CC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 384.64

Physical Properties

Property code	Value	Unit	Source
gf	283.70	kJ/mol	Joback Method
hf	-370.01	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	89.79	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.165		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook
tb	951.54	K	Joback Method
tc	1176.23	K	Joback Method
tf	522.31	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.10	J/mol×K	951.54	Joback Method
cpg	1320.53	J/mol×K	988.99	Joback Method
cpg	1351.64	J/mol×K	1026.44	Joback Method
cpg	1383.79	J/mol×K	1063.89	Joback Method
cpg	1417.31	J/mol×K	1101.33	Joback Method
cpg	1452.57	J/mol×K	1138.78	Joback Method
cpg	1489.90	J/mol×K	1176.23	Joback Method

Sources

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=R215119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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