3,5-Cholestadien-7-one, MO

Inchi: InChI=1S/C28H45NO/c1-19(2)10-9-11-20(3)22-13-14-23-26-24(15-17-28(22,23)5)27(4)1
InchiKey: YIIXEXYTOLDYFP-TXYBNLJASA-N
Formula: C28H45NO
SMILES: CON=C1C=C2C=CCCC2(C)C2CCC3(C)C(C(C)CCCC(C)C)CCC3C12
Mol. weight [g/mol]: 411.66

Physical Properties

Property code	Value	Unit	Source
hf	-368.71	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.806		Crippen Method
mcvol	364.890	ml/mol	McGowan Method
pc	913.29	kPa	Joback Method
rinpol	3104.00		NIST Webbook
rinpol	3104.00		NIST Webbook
rinpol	3104.00		NIST Webbook
tb	983.49	K	Joback Method
tc	1217.72	K	Joback Method

Sources

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=R523103&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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