4-Cholesten-3-one, MO

Inchi: InChI=1S/C28H47NO/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(29-30-6)14-16
InchiKey: ANJYUACJDKITGZ-ZAZWZDAPSA-N
Formula: C28H47NO
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCCC(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 413.68

Physical Properties

Property code	Value	Unit	Source
hf	-426.49	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	8.030		Crippen Method
mcvol	369.190	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	984.33	K	Joback Method
tc	1217.74	K	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=R523183&Units=SI

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