5«beta»-Cholestan-3-one, MO

Inchi: InChI=1S/C28H49NO/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(29-30-6)14-16
InchiKey: CHNBWGCZJBZRBU-YFIPUDFWSA-N
Formula: C28H49NO
SMILES: CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
hf	-493.14	kJ/mol	Joback Method
hvap	80.98	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	8.110		Crippen Method
mcvol	373.490	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	3070.00		NIST Webbook
tb	975.52	K	Joback Method
tc	1206.93	K	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=R523445&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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