anti-4-cholesten-3-one, methyloxime derivative

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	3163.00		NIST Webbook
rinpol	3163.00		NIST Webbook
tb	984.33	K	Joback Method
tc	1217.74	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=R417588&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