5-«alpha»-Pregnan-3-one, MO

Inchi: InChI=1S/C22H37NO/c1-5-15-7-9-19-18-8-6-16-14-17(23-24-4)10-12-22(16,3)20(18)11-1
InchiKey: BPMVIIIFXZWLED-OXQRJJEOSA-N
Formula: C22H37NO
SMILES: CCC1CCC2C3CCC4CC(=NOC)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
hf	-358.74	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	6.058		Crippen Method
mcvol	288.950	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2453.00		NIST Webbook
tb	839.12	K	Joback Method
tc	1075.45	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=R486727&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