4-Pregnen-3,11,20-trione, MO

Inchi: InChI=1S/C24H37N3O3/c1-15(25-28-4)19-9-10-20-18-8-7-16-13-17(26-29-5)11-12-23(16
InchiKey: VHOQRAHXASWUEU-VXPSNPRFSA-N
Formula: C24H37N3O3
SMILES: CON=C1C=C2CCC3C(C(=NOC)CC4(C)C(C(C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 415.57

Physical Properties

Property code	Value	Unit	Source
hf	-484.35	kJ/mol	Joback Method
hvap	86.47	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.202		Crippen Method
mcvol	335.930	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook
tb	1094.25	K	Joback Method
tc	1350.52	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486207&Units=SI
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

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