Pregnanedione, MO TMS

Inchi: InChI=1S/C23H38N2O2/c1-15(24-26-4)19-8-9-20-18-7-6-16-14-17(25-27-5)10-12-22(16,
InchiKey: BRBZYVRSVCPKEU-QFSYNTFFSA-N
Formula: C23H38N2O2
SMILES: CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=NOC)CCC32)C1
Mol. weight [g/mol]: 374.56

Physical Properties

Property code	Value	Unit	Source
hf	-439.17	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2868.00		NIST Webbook
tb	960.98	K	Joback Method
tc	1206.29	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=R250578&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

Latest version available from:

https://www.chemeo.com/cid/12-500-2/Pregnanedione-MO-TMS.pdf

Generated by Cheméo on 2024-10-12 09:14:49.345173838 +0000 UTC m=+3305351.982143087.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.