

5«beta»-Androstan-3«alpha»-ol-11,17-dione, MO

Inchi:	InChI=1S/C21H34N2O3/c1-20-10-9-14(24)11-13(20)5-6-15-16-7-8-18(23-26-4)21(16,2)1
InchiKey:	HHVWPZIVZHPIGJ-TVTLFOCSSA-N
Formula:	C21H34N2O3
SMILES:	CON=C1CC2(C)C(=NOC)CCC2C2CCC3CC(O)CCC3(C)C12
Mol. weight [g/mol]:	362.51

Physical Properties

Property code	Value	Unit	Source
hf	-581.52	kJ/mol	Joback Method
hvap	89.41	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.005		Crippen Method
mcvol	292.280	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2543.00		NIST Webbook
rinpol	2543.00		NIST Webbook
tb	1010.00	K	Joback Method
tc	1248.74	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523405&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

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