

# 5-Androsten-3«beta»-ol-17-one (Dehydroepiandrosterone), MO

**Inchi:** InChI=1S/C20H31NO2/c1-19-10-8-14(22)12-13(19)4-5-15-16-6-7-18(21-23-3)20(16,2)11  
**InchiKey:** BGKXRZGDFUMDSW-RIWSWZRASA-N  
**Formula:** C20H31NO2  
**SMILES:** CON=C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 317.47

## Physical Properties

Property code	Value	Unit	Source
hf	-403.04	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.312		Crippen Method
mcvol	262.340	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2472.00		NIST Webbook
tb	894.35	K	Joback Method
tc	1125.87	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=R523490&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

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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