

5«beta»-Androstan-3«alpha»-ol-17-one (Etiocholanolone), MO

Inchi: InChI=1S/C20H33NO2/c1-19-10-8-14(22)12-13(19)4-5-15-16-6-7-18(21-23-3)20(16,2)11
InchiKey: MQRMZRCQGCVFQ-LDFKKHQ TSA-N
Formula: C₂₀H₃₃NO₂
SMILES: CON=C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 319.48

Physical Properties

Property code	Value	Unit	Source
hf	-469.69	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.392		Crippen Method
mcvol	266.640	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinsol	2448.00		NIST Webbook
tb	885.54	K	Joback Method
tc	1114.90	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
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=R523425&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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