

# Androsta-4-ene-3,17-dione, 1alpha-deuterio-

<b>Inchi:</b>	InChI=1S/C19H26O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)
<b>InchiKey:</b>	AEMFNILZOJDQLW-QOWOAITPSA-N
<b>Formula:</b>	C19H25DO2
<b>SMILES:</b>	CC12CCC3C(CCC4=CC(=O)CCC43C)C1CCC2=O
<b>Mol. weight [g/mol]:</b>	287.41

## Physical Properties

Property code	Value	Unit	Source
gf	48.06	kJ/mol	Joback Method
hf	-394.04	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	65.24	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.087		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
tb	818.02	K	Joback Method
tc	1084.47	K	Joback Method
tf	551.33	K	Joback Method
vc	0.882	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.48	J/molxK	818.02	Joback Method
cpg	830.12	J/molxK	862.43	Joback Method
cpg	856.47	J/molxK	906.84	Joback Method
cpg	882.94	J/molxK	951.24	Joback Method
cpg	909.95	J/molxK	995.65	Joback Method
cpg	937.91	J/molxK	1040.06	Joback Method
cpg	967.22	J/molxK	1084.47	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009860&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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