

# 5«beta»,17«alpha»-Dihydroepitestosterone octadecanoate

Inchi:	InChI=1S/C37H64O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-35(39)40-34-23-22
InchiKey:	KZAUIRNIQLKHJV-FGSFGQHJSA-N
Formula:	C37H64O3
SMILES:	CCCCCCCCCCCCCCCCC(=O)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	556.90

## Physical Properties

Property code	Value	Unit	Source
gf	52.54	kJ/mol	Joback Method
hf	-959.65	kJ/mol	Joback Method
hfus	66.54	kJ/mol	Joback Method
hvap	108.64	kJ/mol	Joback Method
log10ws	-11.69		Crippen Method
logp	10.772		Crippen Method
mcvol	497.760	ml/mol	McGowan Method
pc	608.76	kPa	Joback Method
rinpol	4220.46		NIST Webbook
rinpol	4220.46		NIST Webbook
tb	1224.85	K	Joback Method
tc	1520.00	K	Joback Method
tf	736.37	K	Joback Method
vc	1.919	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2133.25	J/mol×K	1224.85	Joback Method
cpg	2189.93	J/mol×K	1274.04	Joback Method
cpg	2250.01	J/mol×K	1323.23	Joback Method
cpg	2314.20	J/mol×K	1372.42	Joback Method
cpg	2383.25	J/mol×K	1421.62	Joback Method
cpg	2457.86	J/mol×K	1470.81	Joback Method
cpg	2538.75	J/mol×K	1520.00	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=R190397&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190397&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</b>	Non-polar retention indices
<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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