

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

Inchi:	InChI=1S/C26H42O3/c1-4-5-6-7-8-24(28)29-23-12-11-21-20-10-9-18-17-19(27)13-15-25
InchiKey:	DDYHAKNCTGGYOK-FPFLBTHASA-N
Formula:	C26H42O3
SMILES:	CCCCCCC(=O)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	402.61

## Physical Properties

Property code	Value	Unit	Source
gf	-40.08	kJ/mol	Joback Method
hf	-732.61	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.480		Crippen Method
mcvol	342.770	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinsol	3003.52		NIST Webbook
tb	973.17	K	Joback Method
tc	1207.14	K	Joback Method
tf	612.40	K	Joback Method
vc	1.304	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.77	J/mol×K	973.17	Joback Method
cpg	1339.40	J/mol×K	1012.17	Joback Method
cpg	1370.37	J/mol×K	1051.16	Joback Method
cpg	1401.98	J/mol×K	1090.16	Joback Method
cpg	1434.54	J/mol×K	1129.15	Joback Method
cpg	1468.38	J/mol×K	1168.15	Joback Method
cpg	1503.80	J/mol×K	1207.14	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R190377&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190377&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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