5«alpha»,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-XVVWRCIGSA-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
rinpol	3088.48		NIST Webbook
rinpol	3088.48		NIST Webbook
tb	973.17	K	Joback Method
tc	1207.14	K	Joback Method
tf	612.40	K	Joback Method
vc	1.304	m3/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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R190199&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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