5«beta»,17«alpha»-Dihydroepitestosterone dodecanoate

Inchi: InChI=1S/C31H52O3/c1-4-5-6-7-8-9-10-11-12-13-29(33)34-28-17-16-26-25-15-14-23-22

InchiKey: BTKHMAJQYKSLGC-NYFPNFLXSA-N

Formula: C31H52O3

SMILES: CCCCCCCCCCCC(=O)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 472.74

Physical Properties

Property code	Value	Unit	Source
gf	2.02	kJ/mol	Joback Method
hf	-835.81	kJ/mol	Joback Method
hfus	51.00	kJ/mol	Joback Method
hvap	95.29	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.431		Crippen Method
mcvol	413.220	ml/mol	McGowan Method
pc	827.16	kPa	Joback Method
rinpol	3542.61		NIST Webbook
rinpol	3542.61		NIST Webbook
tb	1087.57	K	Joback Method
tc	1331.61	K	Joback Method
tf	668.75	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1666.72	J/mol×K	1087.57	Joback Method
cpg	1704.36	J/mol×K	1128.24	Joback Method
cpg	1743.14	J/mol×K	1168.92	Joback Method
cpg	1783.43	J/mol×K	1209.59	Joback Method
cpg	1825.63	J/mol×K	1250.26	Joback Method
cpg	1870.11	J/mol×K	1290.94	Joback Method
cpg	1917.24	J/mol×K	1331.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190357&Units=SI
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

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