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

Inchi: InChI=1S/C29H48O3/c1-4-5-6-7-8-9-10-11-27(31)32-26-15-14-24-23-13-12-21-20-22(30)

InchiKey: NSSACAVBNVEUOR-ZCNWMKSSSA-N

Formula: C29H48O3

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

Mol. weight [g/mol]: 444.69

Physical Properties

Property code	Value	Unit	Source
gf	-14.82	kJ/mol	Joback Method
hf	-794.53	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.651		Crippen Method
mcvol	385.040	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
rinpol	3323.08		NIST Webbook
tb	1041.81	K	Joback Method
tc	1278.84	K	Joback Method
tf	646.21	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.32	J/mol×K	1041.81	Joback Method
cpg	1554.50	J/mol×K	1081.31	Joback Method
cpg	1589.45	J/mol×K	1120.82	Joback Method
cpg	1625.49	J/mol×K	1160.32	Joback Method
cpg	1662.97	J/mol×K	1199.83	Joback Method
cpg	1702.23	J/mol×K	1239.33	Joback Method
cpg	1743.61	J/mol×K	1278.84	Joback Method

Sources

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=R190342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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