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

Inchi: InChI=1S/C33H56O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-31(35)36-30-19-18-28-27-17-16

InchiKey: KHBHXBFIPLSHCM-NFZKGXJRSA-N

Formula: C33H56O3

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

Mol. weight [g/mol]: 500.80

Physical Properties

Property code	Value	Unit	Source
gf	18.86	kJ/mol	Joback Method
hf	-877.09	kJ/mol	Joback Method
hfus	56.18	kJ/mol	Joback Method
hvap	99.74	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	9.211		Crippen Method
mcvol	441.400	ml/mol	McGowan Method
pc	742.86	kPa	Joback Method
rinpol	3765.97		NIST Webbook
tb	1133.33	K	Joback Method
tc	1388.96	K	Joback Method
tf	691.29	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1817.55	J/mol×K	1133.33	Joback Method
cpg	1859.83	J/mol×K	1175.94	Joback Method
cpg	1903.76	J/mol×K	1218.54	Joback Method
cpg	1949.79	J/mol×K	1261.15	Joback Method
cpg	1998.36	J/mol×K	1303.75	Joback Method
cpg	2049.92	J/mol×K	1346.36	Joback Method
cpg	2104.92	J/mol×K	1388.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190411&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

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