5«alpha»,17«alpha»-Dihydroepitestosterone ethanoate

Inchi: InChI=1S/C21H32O3/c1-13(22)24-19-7-6-17-16-5-4-14-12-15(23)8-10-20(14,2)18(16)9-1

InchiKey: ILCTUFVQFCIIDS-KRXLYJNWSA-N

Formula: C21H32O3

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

Mol. weight [g/mol]: 332.48

Physical Properties

Property code	Value	Unit	Source
gf	-82.18	kJ/mol	Joback Method
hf	-629.41	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	73.03	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.530		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2590.84		NIST Webbook
rinpol	2590.84		NIST Webbook
tb	858.77	K	Joback Method
tc	1104.16	K	Joback Method
tf	556.05	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.38	J/mol×K	858.77	Joback Method
cpg	1004.86	J/mol×K	899.67	Joback Method
cpg	1032.08	J/mol×K	940.57	Joback Method
cpg	1059.38	J/mol×K	981.46	Joback Method
cpg	1087.10	J/mol×K	1022.36	Joback Method
cpg	1115.57	J/mol×K	1063.26	Joback Method
cpg	1145.13	J/mol×K	1104.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190184&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

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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