

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

Inchi: InChI=1S/C37H64O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-35(39)40-34-23-22
InchiKey: KZAUIRNIQLKHJV-CZSVOGOUSA-N
Formula: C37H64O3
SMILES: CCCCCCCCCCCCCCCCCC(=O)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 556.90

Physical Properties

Property code	Value	Unit	Source
gf	52.54	kJ/mol	Joback Method
hf	-959.65	kJ/mol	Joback Method
hfus	66.54	kJ/mol	Joback Method
hvap	108.64	kJ/mol	Joback Method
log10ws	-11.69		Crippen Method
logp	10.772		Crippen Method
mcvol	497.760	ml/mol	McGowan Method
pc	608.76	kPa	Joback Method
rinpol	4313.88		NIST Webbook
tb	1224.85	K	Joback Method
tc	1520.00	K	Joback Method
tf	736.37	K	Joback Method
vc	1.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2133.25	J/mol×K	1224.85	Joback Method
cpg	2189.93	J/mol×K	1274.04	Joback Method
cpg	2250.01	J/mol×K	1323.23	Joback Method
cpg	2314.20	J/mol×K	1372.42	Joback Method
cpg	2383.25	J/mol×K	1421.62	Joback Method
cpg	2457.86	J/mol×K	1470.81	Joback Method
cpg	2538.75	J/mol×K	1520.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R190213&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
hvac:	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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