6,6-Ethylene testosterone 17-cyclopenten-1'-yl ether

Inchi: InChI=1S/C26H36O2/c1-24-11-9-17(27)15-22(24)26(13-14-26)16-19-20-7-8-23(28-18-5-
InchiKey: HRGXQPKZXILWSB-UHFFFAOYSA-N
Formula: C26H36O2
SMILES: CC12CCC(=O)C=C1C1(CC1)CC1C2CCC2(C)C(OC3=CCCC3)CCC12
Mol. weight [g/mol]: 380.56
CAS: 5630-90-0

Physical Properties

Property code	Value	Unit	Source
gf	248.83	kJ/mol	Joback Method
hf	-332.05	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	78.78	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.361		Crippen Method
mcvol	310.880	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
tb	954.91	K	Joback Method
tc	1218.89	K	Joback Method
tf	653.77	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.04	J/mol×K	954.91	Joback Method
cpg	1226.41	J/mol×K	998.91	Joback Method
cpg	1267.28	J/mol×K	1042.90	Joback Method
cpg	1311.37	J/mol×K	1086.90	Joback Method
cpg	1359.37	J/mol×K	1130.90	Joback Method
cpg	1411.97	J/mol×K	1174.89	Joback Method
cpg	1469.89	J/mol×K	1218.89	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=C5630900&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume