3'-(3-Methoxy-1,3,5(10)-estratrien-16beta-yl)propio

Inchi: InChI=1S/C22H28O3/c1-22-10-9-17-16-7-5-15(24-2)11-13(16)3-6-18(17)19(22)12-14-4-8
InchiKey: GJFFFGZCCKLBIO-UHFFFAOYSA-N
Formula: C22H28O3
SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)C1CC1CCC(=O)OC12
Mol. weight [g/mol]: 340.46
CAS: 95809-84-0

Physical Properties

Property code	Value	Unit	Source
gf	99.59	kJ/mol	Joback Method
hf	-438.46	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	77.73	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.483		Crippen Method
mcvol	266.950	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
tb	887.26	K	Joback Method
tc	1140.21	K	Joback Method
tf	582.80	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.92	J/mol×K	887.26	Joback Method
cpg	972.96	J/mol×K	929.42	Joback Method
cpg	996.32	J/mol×K	971.58	Joback Method
cpg	1019.25	J/mol×K	1013.74	Joback Method
cpg	1042.03	J/mol×K	1055.89	Joback Method
cpg	1064.92	J/mol×K	1098.05	Joback Method
cpg	1088.20	J/mol×K	1140.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95809840&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume