3-Methoxy-17beta-formyl-1,3,5(10)-estratriene

Inchi: InChI=1S/C20H26O2/c1-20-10-9-17-16-7-5-15(22-2)11-13(16)3-6-18(17)19(20)8-4-14(20
InchiKey: NMYYLLXEYZDKPO-UHFFFAOYSA-N
Formula: C20H26O2
SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)C(C=O)CCC12
Mol. weight [g/mol]: 298.42
CAS: 63779-92-0

Physical Properties

Property code	Value	Unit	Source
gf	143.29	kJ/mol	Joback Method
hf	-279.70	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.366		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
tb	784.38	K	Joback Method
tc	1020.26	K	Joback Method
tf	493.05	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.22	J/mol×K	784.38	Joback Method
cpg	809.05	J/mol×K	823.69	Joback Method
cpg	829.98	J/mol×K	863.01	Joback Method
cpg	850.26	J/mol×K	902.32	Joback Method
cpg	870.10	J/mol×K	941.64	Joback Method
cpg	889.73	J/mol×K	980.95	Joback Method
cpg	909.39	J/mol×K	1020.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63779920&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume