1,3,5(10)-Oestratrien-17«alpha»-ol, 3-methoxy

Inchi: InChI=1S/C19H26O2/c1-19-10-9-15-14-6-4-13(21-2)11-12(14)3-5-16(15)17(19)7-8-18(19
InchiKey: ULAADVBNYHGIBP-QXCZDIPSSA-N
Formula: C19H26O2
SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	97.57	kJ/mol	Joback Method
hf	-325.71	kJ/mol	Joback Method
hfus	29.55	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.912		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	805.02	K	Joback Method
tc	1027.66	K	Joback Method
tf	500.60	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.05	J/mol×K	805.02	Joback Method
cpg	795.92	J/mol×K	842.13	Joback Method
cpg	815.15	J/mol×K	879.23	Joback Method
cpg	833.91	J/mol×K	916.34	Joback Method
cpg	852.41	J/mol×K	953.45	Joback Method
cpg	870.84	J/mol×K	990.55	Joback Method
cpg	889.38	J/mol×K	1027.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523683&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume