(17«alpha»)-3-Methoxyestra-1,3,5(10)-trien-17-ol

Other names: (17«alpha»)-Estra-1,3,5(10)-triene-3,17-diol
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-UHFFFAOYSA-N
Formula: C19H26O2
SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
hfus	29.55	kJ/mol	Joback Method
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-4.84		Cheméo Relay (1.0)
logp	3.912		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
rinpol	2648.10		NIST Webbook
tf	417.64	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332921&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point