Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17«beta»)-

Other names: Estra-1,3,5(10)-trien-17«beta»-ol, 3-methoxy-
Estradiol 3-methyl ether
17«beta»-Estradiol 3-methyl ether
3-Methoxy-estra-1,3,5(10)-triene-17-«beta»-ol
3-Methoxyestra-1,3,5(10)-trien-17-«beta»-ol
3-Methoxyoestradiol
Oestradiol 3-methyl ether
Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17beta)-
Estra-1,3,5(10)-trien-17beta-ol, 3-methoxy-
17beta-Estradiol 3-methyl ether
3-Methoxyestradiol
3-O-Methylestradiol
17«beta»-Hydroxy-3-methoxyestra-1,3,5(10)-triene
«beta»-Estradiol, 3-methyl ether
(17«beta»)-3-Methoxyestra-1(10),2,4-trien-17-ol
3-Methoxyoestra-1,3,5(10)-trien-17«beta»-ol
NSC 58851

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

CAS: 1035-77-4

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	2656.60		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1035774&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume