

3-Methoxyestra-1,3,5(10),6,8,14-hexaen-17-one

Inchi:	InChI=1S/C19H18O2/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:	GSJXNXTTXUGDFZ-UHFFFAOYSA-N
Formula:	C19H18O2
SMILES:	COc1ccc2c3c(ccc2c1)C1=CCC(=O)C1(C)CC3
Mol. weight [g/mol]:	278.35
CAS:	21513-03-1

Physical Properties

Property code	Value	Unit	Source
gf	203.63	kJ/mol	Joback Method
hf	-90.89	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.157		Crippen Method
mcvol	216.770	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	811.76	K	Joback Method
tc	1069.15	K	Joback Method
tf	564.80	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.79	J/molxK	811.76	Joback Method
cpg	665.99	J/molxK	854.66	Joback Method
cpg	683.81	J/molxK	897.56	Joback Method
cpg	701.50	J/molxK	940.46	Joback Method
cpg	719.33	J/molxK	983.36	Joback Method
cpg	737.56	J/molxK	1026.26	Joback Method
cpg	756.44	J/molxK	1069.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21513031&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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