

Estra-1,3,5(10)-trien-17-one, 3-methoxy-

Other names:	Estrone methyl ether Estrone 3-methyl ether Oestrone methyl ether 3-Methoxyestra-1,3,5(10)-trien-17-one 3-Methoxyestrone 3-Methoxyoestra-1,3,5(10)-trien-17-one 3-O-Methylestrone NSC 88911
Inchi:	InChI=1S/C19H24O2/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:	BCWWDWHFBMPLFQ-UHFFFAOYSA-N
Formula:	C19H24O2
SMILES:	COc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]:	284.39
CAS:	1624-62-0

Physical Properties

Property code	Value	Unit	Source
gf	119.51	kJ/mol	Joback Method
hf	-290.84	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.120		Crippen Method
mcvol	229.670	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2634.80		NIST Webbook
rinpol	2634.80		NIST Webbook
tb	785.33	K	Joback Method
tc	1034.93	K	Joback Method
tf	512.24	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.56	J/mol×K	785.33	Joback Method
cpg	763.96	J/mol×K	826.93	Joback Method
cpg	785.39	J/mol×K	868.53	Joback Method
cpg	806.08	J/mol×K	910.13	Joback Method
cpg	826.26	J/mol×K	951.73	Joback Method
cpg	846.16	J/mol×K	993.33	Joback Method
cpg	866.01	J/mol×K	1034.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1624620&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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