

Estra-4,9,11-trien-3-one, 17-«beta»-hydroxy-

Other names:	ESTRA-4,9,11-TRIEN-3-ONE, 17-HYDROXY-, (17-«beta»)- RU 2341 Trenbolone 17-«beta»-Trenbolone Trienbolone 17«beta»-Hydroxyestra-4,9,11-trien-3-one estra-4,9,11-trien-3-one, 17-hydroxy-, (17beta)- (17beta)-17-hydroxyestra-4,9,11-trien-3-one
Inchi:	InChI=1S/C18H22O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20
InchiKey:	MEHHPFQKXOUFFV-UHFFFAOYSA-N
Formula:	C18H22O2
SMILES:	CC12C=CC3=C4CCC(=O)C=C4CCC3C1CCC2O
Mol. weight [g/mol]:	270.37
CAS:	10161-33-8

Physical Properties

Property code	Value	Unit	Source
gf	79.27	kJ/mol	Joback Method
hf	-290.21	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	78.81	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.329		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2791.40		NIST Webbook
rinpol	2791.40		NIST Webbook
tb	832.21	K	Joback Method
tc	1070.01	K	Joback Method
tf	539.56	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.36	J/mol×K	832.21	Joback Method
cpg	738.46	J/mol×K	871.84	Joback Method
cpg	757.06	J/mol×K	911.48	Joback Method
cpg	775.38	J/mol×K	951.11	Joback Method
cpg	793.64	J/mol×K	990.74	Joback Method
cpg	812.06	J/mol×K	1030.38	Joback Method
cpg	830.85	J/mol×K	1070.01	Joback Method

Sources

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=C10161338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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