

Estra-1,3,5(10),6-tetraene-3,17-diol, (17«beta»)-

Other names:	Estra-1,3,5(10),6-tetraene-3,17«beta»-diol Estra-1,3,5(10),6-tetraene-3,17beta-diol
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:	VVLCELUSWGWMSW-UHFFFAOYSA-N
Formula:	C18H22O2
SMILES:	CC12CCC3C4ccc(O)cc4C=CC3C1CCC2O
Mol. weight [g/mol]:	270.37
CAS:	7291-41-0

Physical Properties

Property code	Value	Unit	Source
gf	79.12	kJ/mol	Joback Method
hf	-280.91	kJ/mol	Joback Method
hfus	33.17	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.690		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	834.52	K	Joback Method
tc	1070.72	K	Joback Method
tf	567.06	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.68	J/mol×K	834.52	Joback Method
cpg	739.13	J/mol×K	873.89	Joback Method
cpg	757.56	J/mol×K	913.25	Joback Method
cpg	776.28	J/mol×K	952.62	Joback Method
cpg	795.58	J/mol×K	991.98	Joback Method
cpg	815.78	J/mol×K	1031.35	Joback Method
cpg	837.17	J/mol×K	1070.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7291410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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