

Estra-1,3,5(10)-trien-3-ol

Other names:	Estrone, 17-deoxy- 17-Deoxyestrone 17-Desoxyestradiol 3-Hydroxyestra-1,3,5(10)-triene 17-Deoxyestradiol 17-Deoxyoestrone OESTRA-1,3,5(10)-TRIEN-3-OL
Inchi:	InChI=1S/C18H24O/c1-18-9-2-3-17(18)16-6-4-12-11-13(19)5-7-14(12)15(16)8-10-18/h5,
InchiKey:	HJKVPZJVVBHWFCQ-WNRNVDISSA-N
Formula:	C18H24O
SMILES:	CC12CCCC1C1CCc3cc(O)ccc3C1CC2
Mol. weight [g/mol]:	256.38
CAS:	53-63-4

Physical Properties

Property code	Value	Unit	Source
gf	193.69	kJ/mol	Joback Method
hf	-166.12	kJ/mol	Joback Method
hfus	26.79	kJ/mol	Joback Method
hvap	70.24	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.638		Crippen Method
mvol	214.010	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2286.00		NIST Webbook
tb	747.85	K	Joback Method
tc	1002.48	K	Joback Method
tf	509.72	K	Joback Method
vc	0.753	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.59	J/mol×K	747.85	Joback Method

cpg	702.32	J/mol×K	790.29	Joback Method
cpg	723.25	J/mol×K	832.73	Joback Method
cpg	743.79	J/mol×K	875.17	Joback Method
cpg	764.31	J/mol×K	917.61	Joback Method
cpg	785.21	J/mol×K	960.04	Joback Method
cpg	806.88	J/mol×K	1002.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53634&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
mvol:	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

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