Estra-1,3,5(10),7-tetraene-3,17-diol, (17«alpha»)-

Other names: «alpha»-Hydroequiline
17 «alpha»-Dihydroequilin
Dihydroequilin
Estra-1,3,5(10),7-tetraene-3,17«alpha»-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: NLLMJANWPUQQTA-UHFFFAOYSA-N

Formula: C18H22O2

SMILES: CC12CCC3C(=CCc4cc(O)ccc43)C1CCC2O

Mol. weight [g/mol]: 270.37

CAS: 651-55-8

Physical Properties

Property code	Value	Unit	Source
gf	77.20	kJ/mol	Joback Method
hf	-272.04	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.529		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	2772.50		NIST Webbook
rinpol	2751.60		NIST Webbook
rinpol	2751.60		NIST Webbook
rinpol	2772.70		NIST Webbook
tb	844.17	K	Joback Method
tc	1081.03	K	Joback Method
tf	583.82	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.00	J/mol×K	844.17	Joback Method

cpg	734.25	J/mol×K	883.65	Joback Method
cpg	752.62	J/mol×K	923.12	Joback Method
cpg	771.42	J/mol×K	962.60	Joback Method
cpg	790.96	J/mol×K	1002.07	Joback Method
cpg	811.54	J/mol×K	1041.55	Joback Method
cpg	833.47	J/mol×K	1081.03	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=C651558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume