Equilin

Other names:	1,3,5,7-Estratetraen-3-ol-17-one
	3-Hydroxyestra-1,3,5(10),7-tetraen-17-one
	3-hydroxyoestra-1,3,5(10),7-tetraen-17-one
	7-Dehydroestrone
	Dihydroequilenin
	Estra-1,3,5(10),7-tetraen-17-one, 3-hydroxy-
Inchi:	InChI=1S/C18H20O2/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:	WKRLQDKEXYKHJB-UHFFFAOYSA-N
Formula:	C18H20O2
SMILES:	CC12CCC3C(=CCc4cc(O)ccc43)C1CCC2=O
Mol. weight [g/mol]:	268.35
CAS:	474-86-2

Physical Properties

Property code	Value	Unit	Source
gf	99.14	kJ/mol	Joback Method
hf	-237.17	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-5.28		Estimated Solubility Method
log10ws	-5.28		Aqueous Solubility Prediction Method
log10ws	-5.28		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.737		Crippen Method
mcvol	211.280	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	2766.10		NIST Webbook
rinpol	2765.40		NIST Webbook
rinpol	2745.30		NIST Webbook
tb	824.48	K	Joback Method
tc	1091.16	K	Joback Method
tf	595.46	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.95	J/mol×K	824.48	Joback Method
cpg	703.18	J/mol×K	868.93	Joback Method
cpg	723.31	J/mol×K	913.37	Joback Method
cpg	743.72	J/mol×K	957.82	Joback Method
cpg	764.81	J/mol×K	1002.27	Joback Method
cpg	786.96	J/mol×K	1046.71	Joback Method
cpg	810.57	J/mol×K	1091.16	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C474862&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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