Equilenin

Other names:	(+)-Equilenin
	3-Hydroxyestra-1,3,5(10),6,8-pentaen-17-one
	3-hydroxyoestra-1,3,5(10),6,8-pentaen-17-one
	Equilenin acetate
	Equilenina
	Equilenine
	Estra-1,3,5(10),6,8-pentaen-17-one, 3-hydroxy-
	Estra-1,3,5,7,9-pentaen-17-one, 3-hydroxy-
	NSC 9901
	d-Equilenin
Inchi:	InChI=1S/C18H18O2/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:	PDRGHUMCVRDZLQ-UHFFFAOYSA-N
Formula:	C18H18O2
SMILES:	CC12CCc3c(ccc4cc(O)ccc34)C1CCC2=O
Mol. weight [g/mol]:	266.33
CAS:	517-09-9

Physical Properties

Property code	Value	Unit	Source
gf	127.18	kJ/mol	Joback Method
hf	-170.52	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	77.01	kJ/mol	Joback Method
log10ws	-5.24		Aqueous Solubility Prediction Method
log10ws	-5.24		Estimated Solubility Method
log10ws	-5.25		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.944		Crippen Method
mcvol	206.980	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	2862.60		NIST Webbook
rinpol	2837.20		NIST Webbook
rinpol	2863.30		NIST Webbook
tb	833.29	K	Joback Method
tc	1102.60	K	Joback Method

tf	531.65	K	Aqueous Solubility Prediction Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.22	J/mol×K	833.29	Joback Method
cpg	669.21	J/mol×K	878.18	Joback Method
cpg	688.36	J/mol×K	923.06	Joback Method
cpg	708.07	J/mol×K	967.95	Joback Method
cpg	728.74	J/mol×K	1012.83	Joback Method
cpg	750.79	J/mol×K	1057.72	Joback Method
cpg	774.61	J/mol×K	1102.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C517099&Units=SI

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

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

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

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