17 «alpha» Dihydroequilenin

Other names: estra-1,3,5,7,9-pentaene-3,17«alpha»-diol
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: RYWZPRVUQHMJFF-ADKAHSJRSA-N
Formula: C18H20O2
SMILES: CC12CCc3c(ccc4cc(O)ccc34)C1CCC2O
Mol. weight [g/mol]: 268.35
CAS: 6639-99-2

Physical Properties

Property code	Value	Unit	Source
gf	105.24	kJ/mol	Joback Method
hf	-205.39	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.736		Crippen Method
mcvol	211.280	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	2854.30		NIST Webbook
rinpol	2854.30		NIST Webbook
rinpol	2873.90		NIST Webbook
rinpol	2887.30		NIST Webbook
tb	852.98	K	Joback Method
tc	1092.15	K	Joback Method
tf	601.34	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.68	J/mol×K	852.98	Joback Method
cpg	699.94	J/mol×K	892.84	Joback Method
cpg	717.54	J/mol×K	932.70	Joback Method
cpg	735.80	J/mol×K	972.57	Joback Method

cpg	755.03	J/mol×K	1012.43	Joback Method
cpg	775.56	J/mol×K	1052.29	Joback Method
cpg	797.70	J/mol×K	1092.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6639992&Units=SI

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