.alpha.-HYDROEQUILINE

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

Physical Properties

Property code	Value	Unit	Source
hfus	31.71	kJ/mol	Joback Method
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.529		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
rinpol	2751.60		NIST Webbook
rinpol	2772.70		NIST Webbook
rinpol	2772.50		NIST Webbook
rinpol	2751.60		NIST Webbook
tf	452.31	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C651558&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point