DESOXY-DIHYDROESTRONE

Other names:	1,3,5(10)-Estratriene-17«beta»-ol
	1,3,5(10)-Oestratrien-17«beta»-ol
	17«beta»-Estradiol, 3-deoxy-
	17«beta»-Hydroxyestra-1,3,5(10)-triene
	3-Deoxy-17«beta»-estradiol
	3-Deoxyestradiol
	Desoxy-dihydroestrone
	Estra-1,3,5(10)-trien-17-ol, (17«beta»)-
	Estradiol, 3-deoxy-
Inchi:	InChI=1S/C18H24O/c1-18-11-10-14-13-5-3-2-4-12(13)6-7-15(14)16(18)8-9-17(18)19/h2-
InchiKey:	MUENRDYXOADTOC-UHFFFAOYSA-N
Formula:	C18H24O
SMILES:	CC12CCC3c4ccccc4CCC3C1CCC2O
Mol. weight [g/mol]:	256.39

Physical Properties

Property code	Value	Unit	Source
hfus	26.17	kJ/mol	Joback Method
log10ws	-4.69		Cheméo Relay (1.0)
logp	3.904		Crippen Method
mcvol	214.010	ml/mol	McGowan Method
rinpol	2218.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2218.00		NIST Webbook
tf	422.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.46	J/mol×K	754.74	Joback Method
cpg	708.37	J/mol×K	792.64	Joback Method
cpg	727.45	J/mol×K	830.55	Joback Method
cpg	745.92	J/mol×K	868.45	Joback Method
cpg	764.01	J/mol×K	906.35	Joback Method

cpg	781.94	J/mol×K	944.26	Joback Method
cpg	799.93	J/mol×K	982.16	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=C2529648&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