Estra-1,3,5(10),6-tetraene-3,17beta-diol

Other names: Estra-1,3,5(10),6-tetraene-3,17«beta»-diol
Estra-1,3,5(10),6-tetraene-3,17beta-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: VVLCELUSWGWMSW-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: CC12CCC3c4ccc(O)cc4C=CC3C1CCC2O
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
hfus	33.17	kJ/mol	Joback Method
log10ws	-4.12		Cheméo Relay (1.0)
logp	3.690		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
tf	465.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.68	J/mol×K	834.52	Joback Method
cpg	739.13	J/mol×K	873.89	Joback Method
cpg	757.56	J/mol×K	913.25	Joback Method
cpg	776.28	J/mol×K	952.62	Joback Method
cpg	795.58	J/mol×K	991.98	Joback Method
cpg	815.78	J/mol×K	1031.35	Joback Method
cpg	837.17	J/mol×K	1070.72	Joback Method

Sources

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=C7291410&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tf:	Normal melting (fusion) point