1,3,5(10)-Oestratrien-17-one

Inchi: InChI=1S/C18H22O/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: LGHBWDKMGOIZKH-LISAXSMJSA-N
Formula: C18H22O
SMILES: CC12CCC3c4ccccc4CCC3C1CCC2=O
Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	225.72	kJ/mol	Joback Method
hf	-126.51	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.112		Crippen Method
mcvol	209.710	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	735.05	K	Joback Method
tc	993.80	K	Joback Method
tf	466.22	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.44	J/mol×K	735.05	Joback Method
cpg	677.32	J/mol×K	778.18	Joback Method
cpg	698.99	J/mol×K	821.30	Joback Method
cpg	719.76	J/mol×K	864.43	Joback Method
cpg	739.89	J/mol×K	907.55	Joback Method
cpg	759.69	J/mol×K	950.68	Joback Method
cpg	779.44	J/mol×K	993.80	Joback Method

Sources

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=R523747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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