Estran-3-one, 17-hydroxy-, (5«alpha»,17«beta»)-

Other names: 5«alpha»-Estran-3-one, 17«beta»-hydroxy-
19-Nor-5«alpha»-dihydrotestosterone
5«alpha»-Estran-3-on-17«beta»-ol
17-Hydroxyestran-3-one-, (5«alpha»,17«beta»)-
5A-Estran-3-on-17B-ol

Inchi: InChI=1S/C18H28O2/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: RHVBIEJVJWNXBU-UHFFFAOYSA-N

Formula: C18H28O2

SMILES: CC12CCC3C4CCC(=O)CC4CCC3C1CCC2O

Mol. weight [g/mol]: 276.41

CAS: 1434-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-4.85	kJ/mol	Joback Method
hf	-490.16	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.569		Crippen Method
mcvol	228.480	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2395.00		NIST Webbook
tb	805.78	K	Joback Method
tc	1036.50	K	Joback Method
tf	487.00	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.75	J/mol×K	805.78	Joback Method
cpg	836.59	J/mol×K	844.23	Joback Method
cpg	858.43	J/mol×K	882.69	Joback Method

cpg	879.47	J/mol×K	921.14	Joback Method
cpg	899.90	J/mol×K	959.59	Joback Method
cpg	919.91	J/mol×K	998.05	Joback Method
cpg	939.69	J/mol×K	1036.50	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=C1434851&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