dehydroepiandrosterone, 3«beta»-hydroxy-5-androstene-17-one

Inchi: InChI=1S/C17H24O2/c18-11-2-4-12-10(9-11)1-3-14-13(12)5-6-16-15(14)7-8-17(16)19/h1

InchiKey: RCKYROOPMBBTQK-WFWUXJIDSA-N

Formula: C17H24O2

SMILES: O=C1CCC2C1CCC1C3CCC(O)CC3=CCC21

Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	20.26	kJ/mol	Joback Method
hf	-418.11	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.099		Crippen Method
mcvol	210.090	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2597.00		NIST Webbook
tb	791.47	K	Joback Method
tc	1021.16	K	Joback Method
tf	469.35	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.36	J/mol×K	791.47	Joback Method
cpg	748.42	J/mol×K	829.75	Joback Method
cpg	767.00	J/mol×K	868.03	Joback Method
cpg	784.20	J/mol×K	906.32	Joback Method
cpg	800.11	J/mol×K	944.60	Joback Method
cpg	814.80	J/mol×K	982.88	Joback Method
cpg	828.37	J/mol×K	1021.16	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=R249033&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