17«alpha»-Hydroxypregnenolone, dimethyl ether

Other names: 3,17-Dimethoxypregn-5-en-20-one
Inchi: InChI=1S/C23H36O3/c1-15(24)23(26-5)13-10-20-18-7-6-16-14-17(25-4)8-11-21(16,2)19
InchiKey: PLULAEHKKBEIQP-UHFFFAOYSA-N
Formula: C23H36O3
SMILES: COC1CCC2(C)C(=CCC3C2CCC2(C)C3CCC2(OC)C(C)=O)C1
Mol. weight [g/mol]: 360.53

Physical Properties

Property code	Value	Unit	Source
gf	-32.91	kJ/mol	Joback Method
hf	-603.66	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.938		Crippen Method
mcvol	300.500	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2805.50		NIST Webbook
rinpol	2805.50		NIST Webbook
tb	863.51	K	Joback Method
tc	1099.10	K	Joback Method
tf	569.78	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.49	J/mol×K	863.51	Joback Method
cpg	1090.19	J/mol×K	902.77	Joback Method
cpg	1120.53	J/mol×K	942.04	Joback Method
cpg	1151.95	J/mol×K	981.30	Joback Method
cpg	1184.87	J/mol×K	1020.57	Joback Method
cpg	1219.72	J/mol×K	1059.83	Joback Method
cpg	1256.93	J/mol×K	1099.10	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=U332965&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