

3Alpha,5alpha-cyclo-17alpha-pregnan-20-one, 6beta-methoxy-

Inchi:	InChI=1S/C22H34O2/c1-13(23)16-5-6-17-15-11-19(24-4)22-12-14(22)7-10-21(22,3)18(1
InchiKey:	PJHBKOQWGPXVAP-UHFFFAOYSA-N
Formula:	C22H34O2
SMILES:	COC1CC2C3CCC(C(C)=O)C3(C)CCC2C2(C)CCC3CC312
Mol. weight [g/mol]:	330.50

Physical Properties

Property code	Value	Unit	Source
gf	132.68	kJ/mol	Joback Method
hf	-426.17	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.859		Crippen Method
mcvol	273.980	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
tb	803.33	K	Joback Method
tc	1037.12	K	Joback Method
tf	547.26	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.08	J/molxK	803.33	Joback Method
cpg	990.15	J/molxK	842.30	Joback Method
cpg	1018.60	J/molxK	881.26	Joback Method
cpg	1047.91	J/molxK	920.23	Joback Method
cpg	1078.58	J/molxK	959.19	Joback Method
cpg	1111.13	J/molxK	998.16	Joback Method
cpg	1146.03	J/molxK	1037.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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