5«beta»-Pregn-7-ene-3«alpha»-ol-20-one

Inchi: InChI=1S/C21H32O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2
InchiKey: DAQICXZASLZNAM-CZTKJMCCSA-N
Formula: C21H32O2
SMILES: CC(=O)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	28.92	kJ/mol	Joback Method
hf	-465.41	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	864.85	K	Joback Method
tc	1091.42	K	Joback Method
tf	539.70	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.54	J/mol×K	864.85	Joback Method
cpg	974.02	J/mol×K	902.61	Joback Method
cpg	998.64	J/mol×K	940.37	Joback Method
cpg	1023.72	J/mol×K	978.14	Joback Method
cpg	1049.57	J/mol×K	1015.90	Joback Method
cpg	1076.50	J/mol×K	1053.66	Joback Method
cpg	1104.85	J/mol×K	1091.42	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=R304046&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