5«beta»-Pregn-8-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: KOMQIFOLNCGLSW-SFRSKELPSA-N
Formula: C21H32O2
SMILES: CC(=O)C1CCC2C3=C(CCC12C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	27.00	kJ/mol	Joback Method
hf	-456.54	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.659		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	874.50	K	Joback Method
tc	1101.93	K	Joback Method
tf	556.46	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.41	J/mol×K	874.50	Joback Method
cpg	970.83	J/mol×K	912.40	Joback Method
cpg	995.53	J/mol×K	950.31	Joback Method
cpg	1020.83	J/mol×K	988.21	Joback Method
cpg	1047.06	J/mol×K	1026.12	Joback Method
cpg	1074.53	J/mol×K	1064.02	Joback Method
cpg	1103.57	J/mol×K	1101.93	Joback Method

Sources

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=R304066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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