Pregnenolone-7,9(11)-dien

Inchi: InChI=1S/C21H28O2/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: UXVHRPVNMQOBJW-UHFFFAOYSA-N
Formula: C21H28O2
SMILES: CC(=O)C1CCC2C3=CC=C4CC(O)CCC4(C)C3=CCC12C
Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
gf	85.00	kJ/mol	Joback Method
hf	-332.11	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.356		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	882.47	K	Joback Method
tc	1113.39	K	Joback Method
tf	574.74	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.42	J/mol×K	882.47	Joback Method
cpg	907.33	J/mol×K	920.96	Joback Method
cpg	930.82	J/mol×K	959.44	Joback Method
cpg	955.23	J/mol×K	997.93	Joback Method
cpg	980.88	J/mol×K	1036.42	Joback Method
cpg	1008.13	J/mol×K	1074.91	Joback Method
cpg	1037.31	J/mol×K	1113.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U214184&Units=SI
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

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