Pregnane-3,20-dione, (5«beta»)-

Other names:	5«beta»-Pregnane-3,20-dione
	5«beta»-Dihydroprogesterone
	5«beta»-Pregnan-3,20-dione
	NSC 82868
	5beta-Pregnan-3,20-dione
	5B-Pregnan-3,20-dione
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:	XMRPGKVKISIQBV-IWQCLKLKSA-N
Formula:	C21H32O2
SMILES:	CC(=O)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	316.48
CAS:	128-23-4

Physical Properties

Property code	Value	Unit	Source
gf	22.82	kJ/mol	Joback Method
hf	-497.19	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.803		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	836.35	K	Joback Method
tc	1084.99	K	Joback Method
tf	473.00 ± 4.00	K	NIST Webbook
tf	393.00 ± 4.00	K	NIST Webbook
tf	565.40 ± 2.00	K	NIST Webbook
tf	472.00 ± 6.00	K	NIST Webbook
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.85	J/mol×K	836.35	Joback Method
cpg	971.72	J/mol×K	877.79	Joback Method
cpg	999.25	J/mol×K	919.23	Joback Method
cpg	1026.83	J/mol×K	960.67	Joback Method
cpg	1054.81	J/mol×K	1002.11	Joback Method
cpg	1083.58	J/mol×K	1043.55	Joback Method
cpg	1113.51	J/mol×K	1084.99	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128234&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

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