

5«alpha»-Dihydroprogesterone

Other names:	5«alpha»-Pregnane-3,20-dione 3,20-Allopregnenedione Pregnane-3,20-dione, (5«alpha»)- 3,20-Dioxo-5«alpha»-pregnane 5«alpha»-Pregnan-3,20-dione Allopregnan-3,20-dione NSC 18319 5A-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-NGEWVIDBSA-N
Formula:	C21H32O2
SMILES:	CC(=O)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	316.48
CAS:	566-65-4

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	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	836.35	K	Joback Method
tc	1084.99	K	Joback Method
tf	533.82	K	Joback Method
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

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=C566654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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