

Pregnan-3-one, 20-hydroxy-, (5«alpha»,20R)-

Other names:	Allopregnan-20«beta»-ol-3-one 5«alpha»-pregnan-20«BETA»-ol-3-one
Inchi:	InChI=1S/C21H34O2/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:	DYVGYXXLXQESJE-FWWCHYQUSA-N
Formula:	C21H34O2
SMILES:	CC(O)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	318.49
CAS:	516-58-5

Physical Properties

Property code	Value	Unit	Source
gf	12.48	kJ/mol	Joback Method
hf	-542.12	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.595		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
tb	874.22	K	Joback Method
tc	1105.78	K	Joback Method
tf	468.00 ± 3.00	K	NIST Webbook
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.23	J/mol×K	874.22	Joback Method
cpg	1023.60	J/mol×K	912.81	Joback Method
cpg	1049.94	J/mol×K	951.41	Joback Method
cpg	1076.57	J/mol×K	990.00	Joback Method
cpg	1103.80	J/mol×K	1028.59	Joback Method
cpg	1131.92	J/mol×K	1067.18	Joback Method
cpg	1161.26	J/mol×K	1105.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C516585&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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