

11 «alpha»-Hydroxyprogesterone, methyl ether

Other names:	(11 «alpha»)-11-Methoxypregn-4-ene-3,20-dione
Inchi:	InChI=1S/C22H32O3/c1-13(23)17-7-8-18-16-6-5-14-11-15(24)9-10-21(14,2)20(16)19(25)
InchiKey:	IIAUVJAANFPGEA-UHFFFAOYSA-N
Formula:	C22H32O3
SMILES:	<chem>COC1CC2(C)C(C(C)=O)CCC2C2CCC3=CC(=O)CCC3(C)C12</chem>
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-53.43	kJ/mol	Joback Method
hf	-603.74	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.348		Crippen Method
mvol	282.110	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	3015.70		NIST Webbook
tb	885.79	K	Joback Method
tc	1129.77	K	Joback Method
tf	580.60	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.39	J/mol×K	885.79	Joback Method
cpg	1039.66	J/mol×K	926.45	Joback Method
cpg	1066.89	J/mol×K	967.12	Joback Method
cpg	1094.43	J/mol×K	1007.78	Joback Method
cpg	1122.58	J/mol×K	1048.44	Joback Method
cpg	1151.68	J/mol×K	1089.11	Joback Method
cpg	1182.06	J/mol×K	1129.77	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=U332961&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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