

Pregn-4-ene-3,20-dione, 16,17-epoxy-, (16«alpha»)-

Other names:	Pregn-4-ene-3,20-dione, 16-«alpha»,17-epoxy- 16-«alpha»,17-Epoxypregn-4-ene-3,20-dione 16«alpha»,17«alpha»-Epoxypregn-4-ene-3,20-dione 16«alpha»,17«alpha»-epoxyprogesterone
Inchi:	InChI=1S/C21H28O3/c1-12(22)21-18(24-21)11-17-15-5-4-13-10-14(23)6-8-19(13,2)16(1
InchiKey:	LHNVKVKZPHUYQO-UHFFFAOYSA-N
Formula:	C21H28O3
SMILES:	CC(=O)C12OC1CC1C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	328.45
CAS:	1097-51-4

Physical Properties

Property code	Value	Unit	Source
gf	44.20	kJ/mol	Joback Method
hf	-462.18	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.855		Crippen Method
mcvol	257.160	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	870.55	K	Joback Method
tc	1126.69	K	Joback Method
tf	626.79	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.37	J/mol×K	1084.00	Joback Method
cpg	921.39	J/mol×K	870.55	Joback Method
cpg	950.56	J/mol×K	913.24	Joback Method
cpg	981.32	J/mol×K	955.93	Joback Method
cpg	1014.29	J/mol×K	998.62	Joback Method

cpg	1050.10	J/mol×K	1041.31	Joback Method
cpg	1132.72	J/mol×K	1126.69	Joback Method
hfust	26.40	kJ/mol	328.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1097514&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
hfust:	Enthalpy of fusion at a given temperature
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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