5-«alpha»-Pregnane-20-«alpha»,21-diol, diacetate

Inchi: InChI=1S/C25H40O4/c1-16(26)28-15-23(29-17(2)27)22-11-10-20-19-9-8-18-7-5-6-13-24

InchiKey: RZMRLFZKLOVKNA-SUSDATBNSA-N

Formula: C25H40O4

SMILES: CC(=O)OCC(OC(C)=O)C1CCC2C3CCC4CCCCC4(C)C3CCC12C

Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-162.27	kJ/mol	Joback Method
hf	-824.35	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	86.45	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.530		Crippen Method
mcvol	334.550	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	958.32	K	Joback Method
tc	1191.49	K	Joback Method
tf	590.07	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.70	J/mol×K	958.32	Joback Method
cpg	1285.02	J/mol×K	997.18	Joback Method
cpg	1314.70	J/mol×K	1036.04	Joback Method
cpg	1345.04	J/mol×K	1074.90	Joback Method
cpg	1376.39	J/mol×K	1113.76	Joback Method
cpg	1409.05	J/mol×K	1152.62	Joback Method
cpg	1443.35	J/mol×K	1191.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149874&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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