

5-Pregnene-3«beta»,20«beta»,21-triol, triacetate

Inchi:	InChI=1S/C27H40O6/c1-16(28)31-15-25(33-18(3)30)24-9-8-22-21-7-6-19-14-20(32-17(2
InchiKey:	SZFAWVIPSFYGQF-NIHJCPRLSA-N
Formula:	C27H40O6
SMILES:	CC(=O)OCC(OC(C)=O)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	460.60

Physical Properties

Property code	Value	Unit	Source
gf	-359.02	kJ/mol	Joback Method
hf	-1064.12	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.992		Crippen Method
mcvol	365.870	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinsol	3225.00		NIST Webbook
tb	1084.51	K	Joback Method
tc	1330.40	K	Joback Method
tf	698.05	K	Joback Method
vc	1.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.63	J/molxK	1084.51	Joback Method
cpg	1461.35	J/molxK	1125.49	Joback Method
cpg	1495.29	J/molxK	1166.47	Joback Method
cpg	1530.81	J/molxK	1207.46	Joback Method
cpg	1568.27	J/molxK	1248.44	Joback Method
cpg	1608.01	J/molxK	1289.42	Joback Method
cpg	1650.39	J/molxK	1330.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528915&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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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