

5-«alpha»-Pregnane-17-«alpha»,20-«beta»,21-triol

triacetate

InChI: InChI=1S/C27H42O6/c1-17(28)31-16-24(32-18(2)29)27(33-19(3)30)15-12-23-21-10-9-20

InChIKey:

CVYWPWXPCMXSNC-NKBZBIEASA-N

Formula:

C27H42O6

SMILES:

CC(=O)OCC(OC(C)=O)C1(OC(C)=O)CCC2C3CCC4CCCCC4(C)C3CCC21C

Mol. weight [g/mol]:

462.62

Physical Properties

Property code	Value	Unit	Source
gf	-384.84	kJ/mol	Joback Method
hf	-1095.19	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	98.91	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.216		Crippen Method
mcvol	370.170	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	3005.00		NIST Webbook
tb	1080.61	K	Joback Method
tc	1327.18	K	Joback Method
tf	708.67	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.83	J/molxK	1080.61	Joback Method
cpg	1522.51	J/molxK	1121.70	Joback Method
cpg	1566.94	J/molxK	1162.80	Joback Method
cpg	1614.61	J/molxK	1203.89	Joback Method
cpg	1666.02	J/molxK	1244.99	Joback Method
cpg	1721.65	J/molxK	1286.08	Joback Method
cpg	1781.98	J/molxK	1327.18	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=R149790&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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