17«alpha»,20«beta»,21-Trihydroxypregn-4-en-3-o acetonide

Inchi: InChI=1S/C24H36O4/c1-21(2)27-14-20(28-21)24(26)12-9-19-17-6-5-15-13-16(25)7-10-2

InchiKey: KJLQBUCRDREEMB-CVXBYTLUSA-N

Formula: C24H36O4

SMILES: CC1(C)OCC(C2(O)CCC3C4CCC5=CC(=O)CCC5(C)C4CCC32C)O1

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-86.16	kJ/mol	Joback Method
hf	-725.49	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	95.16	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.401		Crippen Method
mcvol	309.600	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3015.00		NIST Webbook
tb	1017.10	K	Joback Method
tc	1269.86	K	Joback Method
tf	703.64	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.55	J/mol×K	1017.10	Joback Method
cpg	1302.17	J/mol×K	1059.23	Joback Method
cpg	1350.88	J/mol×K	1101.35	Joback Method
cpg	1404.38	J/mol×K	1143.48	Joback Method
cpg	1463.33	J/mol×K	1185.61	Joback Method
cpg	1528.44	J/mol×K	1227.73	Joback Method
cpg	1600.38	J/mol×K	1269.86	Joback Method

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=R524993&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
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