

Pregna-1,4-dien-3-one, 11beta,17alpha,20,21-tetrahydroxy-, 21-acetate

InChI: InChI=1S/C23H32O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14)

InchiKey: TYKFSLOWQCQNQJ-MXUWMZRMSA-N

Formula: C23H32O6

SMILES: CC(=O)OCC(O)C1(O)CCC2C3CCC4=CC(=O)C=CC4(C)C3C(O)CC21C

Mol. weight [g/mol]: 404.50

Physical Properties

Property code	Value	Unit	Source
gf	-433.44	kJ/mol	Joback Method
hf	-1013.33	kJ/mol	Joback Method
hfus	34.78	kJ/mol	Joback Method
hvap	127.22	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	1.920		Crippen Method
mcvol	309.510	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
tb	1184.17	K	Joback Method
tc	1454.37	K	Joback Method
tf	783.99	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.83	J/molxK	1184.17	Joback Method
cpg	1400.90	J/molxK	1229.20	Joback Method
cpg	1459.34	J/molxK	1274.24	Joback Method
cpg	1523.78	J/molxK	1319.27	Joback Method
cpg	1594.86	J/molxK	1364.30	Joback Method
cpg	1673.21	J/molxK	1409.34	Joback Method
cpg	1759.45	J/molxK	1454.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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