

Spiro[cyclopropane-1,6'-[17alpha]pregn-4'-ene]-2'-one, 17'beta-hydroxy-3'-oxo-, gamma-lactone

InChI: InChI=1S/C24H32O3/c1-21-7-3-15(25)13-19(21)23(11-12-23)14-16-17(21)4-8-22(2)18(1)
InChIKey: VN5GXPUCNIQYMW-UHFFFAOYSA-N

Formula: C₂₄H₃₂O₃
SMILES: CC12CCC(=O)C=C1C1(CC1)CC1C2CCC2(C)C1CCC21CCC(=O)O1
Mol. weight [g/mol]: 368.51
CAS: 6987-59-3

Physical Properties

Property code	Value	Unit	Source
gf	114.56	kJ/mol	Joback Method
hf	-453.16	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.984		Crippen Method
mcvol	288.570	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
tb	973.33	K	Joback Method
tc	1254.16	K	Joback Method
tf	717.93	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.65	J/molxK	973.33	Joback Method
cpg	1184.53	J/molxK	1020.13	Joback Method
cpg	1235.31	J/molxK	1066.94	Joback Method
cpg	1292.02	J/molxK	1113.74	Joback Method
cpg	1355.64	J/molxK	1160.55	Joback Method
cpg	1427.18	J/molxK	1207.35	Joback Method
cpg	1507.64	J/molxK	1254.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6987593&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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