Androsta-1,4-diene-16beta-propionic acid, 17beta-hydroxy-3-oxo-, delta-lactone

Inchi: InChI=1S/C22H28O3/c1-21-9-7-15(23)12-14(21)4-5-16-17(21)8-10-22(2)18(16)11-13-3-6

InchiKey: QLYHBVWSOGXASK-UHFFFAOYSA-N

Formula: C22H28O3

SMILES: CC12C=CC(=O)C=C1CCC1C2CCC2(C)C1CC1CCC(=O)OC12

Mol. weight [g/mol]: 340.46

CAS: 95809-79-3

Physical Properties

Property code	Value	Unit	Source
gf	58.10	kJ/mol	Joback Method
hf	-483.88	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.226		Crippen Method
mcvol	266.950	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
tb	919.11	K	Joback Method
tc	1189.08	K	Joback Method
tf	622.65	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.75	J/mol×K	919.11	Joback Method
cpg	1020.08	J/mol×K	964.11	Joback Method
cpg	1049.90	J/mol×K	1009.10	Joback Method
cpg	1080.68	J/mol×K	1054.10	Joback Method
cpg	1112.87	J/mol×K	1099.09	Joback Method
cpg	1146.96	J/mol×K	1144.09	Joback Method
cpg	1183.41	J/mol×K	1189.08	Joback Method

Sources

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=C95809793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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