Androst-4-ene-16beta-proionic acid, 17beta-hydroxy-3-oxo-, delta-lactone

Inchi: InChI=1S/C22H30O3/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: XUYYCWWWEACBMI-UHFFFAOYSA-N

Formula: C22H30O3

SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CC1CCC(=O)OC12

Mol. weight [g/mol]: 342.47

CAS: 96065-28-0

Physical Properties

Property code	Value	Unit	Source
gf	28.14	kJ/mol	Joback Method
hf	-541.66	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.450		Crippen Method
mcvol	271.250	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
tb	919.95	K	Joback Method
tc	1187.87	K	Joback Method
tf	621.89	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1021.00	J/mol×K	919.95	Joback Method
cpg	1051.04	J/mol×K	964.60	Joback Method
cpg	1081.47	J/mol×K	1009.26	Joback Method
cpg	1112.74	J/mol×K	1053.91	Joback Method
cpg	1145.31	J/mol×K	1098.56	Joback Method
cpg	1179.63	J/mol×K	1143.22	Joback Method
cpg	1216.15	J/mol×K	1187.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96065280&Units=SI
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

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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