

Estr-4-ene-16beta-propionic acid, 17beta-hydroxy-3-oxo-, delta-lactone

Inchi:	InChI=1S/C21H28O3/c1-21-9-8-16-15-6-4-14(22)10-12(15)2-5-17(16)18(21)11-13-3-7-19
InchiKey:	RKOYUTWZQGBFLZ-UHFFFAOYSA-N
Formula:	C21H28O3
SMILES:	CC12CCC3C4CCC(=O)C=C4CCC3C1CC1CCC(=O)OC12
Mol. weight [g/mol]:	328.45
CAS:	94962-51-3

Physical Properties

Property code	Value	Unit	Source
gf	25.21	kJ/mol	Joback Method
hf	-536.26	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.060		Crippen Method
mcvol	257.160	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
tb	896.83	K	Joback Method
tc	1161.84	K	Joback Method
tf	586.72	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.94	J/molxK	896.83	Joback Method
cpg	983.51	J/molxK	941.00	Joback Method
cpg	1008.10	J/molxK	985.17	Joback Method
cpg	1031.99	J/molxK	1029.34	Joback Method
cpg	1055.47	J/molxK	1073.50	Joback Method
cpg	1078.80	J/molxK	1117.67	Joback Method
cpg	1102.27	J/molxK	1161.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C94962513&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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