Estrone, butyrate

Inchi: InChI=1S/C22H28O3/c1-3-4-21(24)25-15-6-8-16-14(13-15)5-7-18-17(16)11-12-22(2)19(1
InchiKey: MLGJBWKOEOTZIL-UHFFFAOYSA-N
Formula: C22H28O3
SMILES: CCCC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]: 340.46

Physical Properties

Property code	Value	Unit	Source
gf	15.85	kJ/mol	Joback Method
hf	-465.34	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.817		Crippen Method
mcvol	273.510	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	907.84	K	Joback Method
tc	1149.77	K	Joback Method
tf	595.98	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.76	J/mol×K	907.84	Joback Method
cpg	965.68	J/mol×K	948.16	Joback Method
cpg	987.08	J/mol×K	988.48	Joback Method
cpg	1008.20	J/mol×K	1028.81	Joback Method
cpg	1029.25	J/mol×K	1069.13	Joback Method
cpg	1050.45	J/mol×K	1109.45	Joback Method
cpg	1072.02	J/mol×K	1149.77	Joback Method

Sources

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=U368355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume