Estrone, octanoate

Inchi: InChI=1S/C26H36O3/c1-3-4-5-6-7-8-25(28)29-19-10-12-20-18(17-19)9-11-22-21(20)15-1
InchiKey: QWDKZLPKJDGSQR-UHFFFAOYSA-N
Formula: C26H36O3
SMILES: CCCCCCCC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]: 396.56

Physical Properties

Property code	Value	Unit	Source
gf	49.53	kJ/mol	Joback Method
hf	-547.90	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.378		Crippen Method
mcvol	329.870	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2851.00		NIST Webbook
rinpol	2851.00		NIST Webbook
tb	999.36	K	Joback Method
tc	1235.59	K	Joback Method
tf	641.06	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.10	J/mol×K	999.36	Joback Method
cpg	1223.03	J/mol×K	1038.73	Joback Method
cpg	1246.72	J/mol×K	1078.10	Joback Method
cpg	1270.40	J/mol×K	1117.47	Joback Method
cpg	1294.30	J/mol×K	1156.84	Joback Method
cpg	1318.64	J/mol×K	1196.22	Joback Method
cpg	1343.63	J/mol×K	1235.59	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=U368358&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