Estrone, 4-chlorobutyrate

Inchi: InChI=1S/C22H27ClO3/c1-22-11-10-17-16-7-5-15(26-21(25)3-2-12-23)13-14(16)4-6-18(1
InchiKey: XPAMBWLTGQHJOC-UHFFFAOYSA-N
Formula: C22H27ClO3
SMILES: CC12CCC3c4ccc(OC(=O)CCCCl)cc4CCC3C1CCC2=O
Mol. weight [g/mol]: 374.90

Physical Properties

Property code	Value	Unit	Source
gf	3.92	kJ/mol	Joback Method
hf	-481.08	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	84.58	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.036		Crippen Method
mcvol	285.750	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	945.27	K	Joback Method
tc	1189.92	K	Joback Method
tf	625.90	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.80	J/mol×K	945.27	Joback Method
cpg	994.17	J/mol×K	986.05	Joback Method
cpg	1015.25	J/mol×K	1026.82	Joback Method
cpg	1036.28	J/mol×K	1067.60	Joback Method
cpg	1057.48	J/mol×K	1108.37	Joback Method
cpg	1079.08	J/mol×K	1149.15	Joback Method
cpg	1101.32	J/mol×K	1189.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368357&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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