Estradiol dipropionate

Inchi: InChI=1S/C24H32O4/c1-4-22(25)27-16-7-9-17-15(14-16)6-8-19-18(17)12-13-24(3)20(19
InchiKey: JQIYNMYZKRGDFK-UHFFFAOYSA-N
Formula: C24H32O4
SMILES: CCC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(OC(=O)CC)CCC12
Mol. weight [g/mol]: 384.51
CAS: 309267-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-86.35	kJ/mol	Joback Method
hf	-634.06	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.180		Crippen Method
mcvol	307.560	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
tb	957.40	K	Joback Method
tc	1190.51	K	Joback Method
tf	618.22	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.10	J/mol×K	957.40	Joback Method
cpg	1109.25	J/mol×K	996.25	Joback Method
cpg	1131.06	J/mol×K	1035.10	Joback Method
cpg	1152.76	J/mol×K	1073.95	Joback Method
cpg	1174.55	J/mol×K	1112.80	Joback Method
cpg	1196.64	J/mol×K	1151.66	Joback Method
cpg	1219.26	J/mol×K	1190.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C309267990&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