Androst-5-ene-17,17-ethylenedioxy-3b-hydroxy-,p

Inchi: InChI=1S/C28H35NO6/c1-26-12-9-21(35-25(30)18-3-6-20(7-4-18)29(31)32)17-19(26)5-8
InchiKey: ARNUAHHGHXAYII-UHFFFAOYSA-N
Formula: C28H35NO6
SMILES: CC12CCC(OC(=O)c3ccc([N+](=O)[O-])cc3)CC1=CCC1C2CCC2(C)C1CCC21OCCO1
Mol. weight [g/mol]: 481.58
CAS: 125567-35-3

Physical Properties

Property code	Value	Unit	Source
gf	136.64	kJ/mol	Joback Method
hf	-537.36	kJ/mol	Joback Method
hfus	54.19	kJ/mol	Joback Method
hvap	113.11	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	5.826		Crippen Method
mcvol	359.620	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
tb	1208.57	K	Joback Method
tc	1494.75	K	Joback Method
tf	858.25	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1568.27	J/mol×K	1208.57	Joback Method
cpg	1634.13	J/mol×K	1256.27	Joback Method
cpg	1707.48	J/mol×K	1303.96	Joback Method
cpg	1789.22	J/mol×K	1351.66	Joback Method
cpg	1880.25	J/mol×K	1399.36	Joback Method
cpg	1981.48	J/mol×K	1447.05	Joback Method
cpg	2093.83	J/mol×K	1494.75	Joback Method

Sources

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=C125567353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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