17-Ethylenedioxy-androst-5-en-3beta-ol

Inchi: InChI=1S/C21H32O3/c1-19-8-5-15(22)13-14(19)3-4-16-17(19)6-9-20(2)18(16)7-10-21(20
InchiKey: SXXRMGBMPQWUTB-UHFFFAOYSA-N
Formula: C21H32O3
SMILES: CC12CCC(O)CC1=CCC1C2CCC2(C)C1CCC21OCCO1
Mol. weight [g/mol]: 332.48
CAS: 7745-40-6

Physical Properties

Property code	Value	Unit	Source
gf	36.47	kJ/mol	Joback Method
hf	-514.61	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.053		Crippen Method
mcvol	265.760	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
tb	880.80	K	Joback Method
tc	1121.21	K	Joback Method
tf	585.47	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.80	J/mol×K	880.80	Joback Method
cpg	1009.55	J/mol×K	920.87	Joback Method
cpg	1039.64	J/mol×K	960.94	Joback Method
cpg	1071.61	J/mol×K	1001.00	Joback Method
cpg	1105.98	J/mol×K	1041.07	Joback Method
cpg	1143.28	J/mol×K	1081.14	Joback Method
cpg	1184.04	J/mol×K	1121.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7745406&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