2,5-Seco-a,a-dinor-5beta-androstane-2,5,17beta-tr

Inchi: InChI=1S/C17H30O3/c1-16-8-7-13-11(12(16)4-6-15(16)20)3-5-14(19)17(13,2)9-10-18/h1
InchiKey: LWALRQNSMBJKQV-UHFFFAOYSA-N
Formula: C17H30O3
SMILES: CC1(CCO)C(O)CCC2C1CCC1(C)C(O)CCC21
Mol. weight [g/mol]: 282.42
CAS: 3523-67-9

Physical Properties

Property code	Value	Unit	Source
gf	-226.17	kJ/mol	Joback Method
hf	-708.02	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	100.36	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.333		Crippen Method
mcvol	235.420	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
tb	884.00	K	Joback Method
tc	1087.86	K	Joback Method
tf	534.39	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.21	J/mol×K	884.00	Joback Method
cpg	889.50	J/mol×K	917.98	Joback Method
cpg	910.07	J/mol×K	951.95	Joback Method
cpg	931.11	J/mol×K	985.93	Joback Method
cpg	952.84	J/mol×K	1019.90	Joback Method
cpg	975.46	J/mol×K	1053.88	Joback Method
cpg	999.19	J/mol×K	1087.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3523679&Units=SI

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