3Alpha,5alpha-cycloandrostan-6beta-ol,17-ethyle

Inchi: InChI=1S/C21H32O3/c1-18-6-3-13-12-20(13,18)17(22)11-14-15(18)4-7-19(2)16(14)5-8-2
InchiKey: QKKPKPKZZIQUSI-UHFFFAOYSA-N
Formula: C21H32O3
SMILES: CC12CCC3C(CC(O)C45CC4CCC35C)C1CCC21OCCO1
Mol. weight [g/mol]: 332.48

Physical Properties

Property code	Value	Unit	Source
gf	99.99	kJ/mol	Joback Method
hf	-474.74	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	82.50	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.743		Crippen Method
mcvol	259.200	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
tb	866.16	K	Joback Method
tc	1105.66	K	Joback Method
tf	620.35	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.20	J/mol×K	866.16	Joback Method
cpg	1010.12	J/mol×K	906.08	Joback Method
cpg	1043.42	J/mol×K	945.99	Joback Method
cpg	1079.80	J/mol×K	985.91	Joback Method
cpg	1119.97	J/mol×K	1025.82	Joback Method
cpg	1164.62	J/mol×K	1065.74	Joback Method
cpg	1214.48	J/mol×K	1105.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005240&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume