17-Ethylenedioxy-3alpha,5alpha-cycloandrostan-6

Inchi: InChI=1S/C21H30O3/c1-18-6-3-13-12-20(13,18)17(22)11-14-15(18)4-7-19(2)16(14)5-8-21OCCO1
InchiKey: NXSCSOGTZCZFAL-UHFFFAOYSA-N
Formula: C21H30O3
SMILES: CC12CCC3C(CC(=O)C45CC4CCC35C)C1CCC21OCCO1
Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	121.93	kJ/mol	Joback Method
hf	-439.87	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.951		Crippen Method
mcvol	254.900	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
tb	846.47	K	Joback Method
tc	1115.44	K	Joback Method
tf	631.99	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.54	J/mol×K	846.47	Joback Method
cpg	973.93	J/mol×K	891.30	Joback Method
cpg	1009.87	J/mol×K	936.13	Joback Method
cpg	1049.28	J/mol×K	980.95	Joback Method
cpg	1093.12	J/mol×K	1025.78	Joback Method
cpg	1142.33	J/mol×K	1070.61	Joback Method
cpg	1197.86	J/mol×K	1115.44	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=B6005336&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