5B-Estran-3B,17B-diol, 17A-ethyl

Inchi: InChI=1S/C20H34O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(1
InchiKey: GUBNWXDDDXQJOQ-BUYWQYGGSA-N
Formula: C20H34O2
SMILES: CCC1(O)CCC2C3CCC4CC(O)CCC4C3CCC21C
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	-15.44	kJ/mol	Joback Method
hf	-551.07	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	90.45	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.141		Crippen Method
mcvol	260.960	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	871.47	K	Joback Method
tc	1084.67	K	Joback Method
tf	521.80	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.48	J/mol×K	871.47	Joback Method
cpg	994.25	J/mol×K	907.00	Joback Method
cpg	1018.13	J/mol×K	942.54	Joback Method
cpg	1042.37	J/mol×K	978.07	Joback Method
cpg	1067.25	J/mol×K	1013.60	Joback Method
cpg	1093.02	J/mol×K	1049.14	Joback Method
cpg	1119.95	J/mol×K	1084.67	Joback Method

Sources

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=R5608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume