Estran-4-on-17B-ol, 17-A-methyl

Inchi: InChI=1S/C19H30O2/c1-18-10-8-13-12-4-3-5-17(20)15(12)7-6-14(13)16(18)9-11-19(18,2
InchiKey: LSBJYMKOURZLOC-YOWCBUAKSA-N
Formula: C19H30O2
SMILES: CC1(O)CCC2C3CCC4C(=O)CCCC4C3CCC21C
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	-1.92	kJ/mol	Joback Method
hf	-495.56	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.959		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	828.90	K	Joback Method
tc	1062.98	K	Joback Method
tf	522.17	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.61	J/mol×K	828.90	Joback Method
cpg	895.49	J/mol×K	867.91	Joback Method
cpg	920.14	J/mol×K	906.93	Joback Method
cpg	944.87	J/mol×K	945.94	Joback Method
cpg	969.98	J/mol×K	984.95	Joback Method
cpg	995.80	J/mol×K	1023.97	Joback Method
cpg	1022.62	J/mol×K	1062.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R5679&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume