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

Inchi: InChI=1S/C20H32O2/c1-3-20(22)12-10-17-15-7-8-16-13(5-4-6-18(16)21)14(15)9-11-19(1
InchiKey: PZXUCTNTGYRTTC-JJVWSAESSA-N
Formula: C20H32O2
SMILES: CCC1(O)CCC2C3CCC4C(=O)CCCC4C3CCC21C
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	6.50	kJ/mol	Joback Method
hf	-516.20	kJ/mol	Joback Method
hfus	23.81	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.349		Crippen Method
mcvol	256.660	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	851.78	K	Joback Method
tc	1082.72	K	Joback Method
tf	533.44	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.14	J/mol×K	851.78	Joback Method
cpg	958.57	J/mol×K	890.27	Joback Method
cpg	983.88	J/mol×K	928.76	Joback Method
cpg	1009.37	J/mol×K	967.25	Joback Method
cpg	1035.35	J/mol×K	1005.74	Joback Method
cpg	1062.10	J/mol×K	1044.23	Joback Method
cpg	1089.95	J/mol×K	1082.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R5666&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

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

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