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

Inchi: InChI=1S/C18H30O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20
InchiKey: QNKATSBSLLYTMH-WZCXBNJESA-N
Formula: C18H30O2
SMILES: CC12CCC3C4CCC(O)CC4CCC3C1CCC2O
Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
gf	-26.79	kJ/mol	Joback Method
hf	-525.03	kJ/mol	Joback Method
hfus	30.58	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.361		Crippen Method
mcvol	232.780	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2390.00		NIST Webbook
tb	825.47	K	Joback Method
tc	1035.67	K	Joback Method
tf	475.36	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.48	J/mol×K	825.47	Joback Method
cpg	870.13	J/mol×K	860.50	Joback Method
cpg	890.09	J/mol×K	895.54	Joback Method
cpg	909.51	J/mol×K	930.57	Joback Method
cpg	928.58	J/mol×K	965.60	Joback Method
cpg	947.46	J/mol×K	1000.64	Joback Method
cpg	966.32	J/mol×K	1035.67	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=R5580&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