5«alpha»-Oestrane

Inchi: InChI=1S/C18H30/c1-18-11-4-7-17(18)16-9-8-13-5-2-3-6-14(13)15(16)10-12-18/h13-17H
InchiKey: GRXPVLPQNMUNNX-SNMURISASA-N
Formula: C18H30
SMILES: CC12CCCC1C1CCC3CCCCC3C1CC2
Mol. weight [g/mol]: 246.43

Physical Properties

Property code	Value	Unit	Source
gf	262.27	kJ/mol	Joback Method
hf	-179.89	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.419		Crippen Method
mcvol	221.040	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	650.45	K	Joback Method
tc	890.00	K	Joback Method
tf	362.20	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.72	J/mol×K	650.45	Joback Method
cpg	715.69	J/mol×K	690.38	Joback Method
cpg	742.77	J/mol×K	730.30	Joback Method
cpg	768.23	J/mol×K	770.23	Joback Method
cpg	792.33	J/mol×K	810.15	Joback Method
cpg	815.33	J/mol×K	850.08	Joback Method
cpg	837.50	J/mol×K	890.00	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=R523970&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