Epitostanol

Other names: epitiostanol
Inchi: InChI=1S/C19H30OS/c1-18-8-7-14-12(13(18)5-6-17(18)20)4-3-11-9-15-16(21-15)10-19(1
InchiKey: OBMLHUPNRURLOK-UHFFFAOYSA-N
Formula: C19H30OS
SMILES: CC12CCC3C(CCC4CC5SC5CC43C)C1CCC2O
Mol. weight [g/mol]: 306.51

Physical Properties

Property code	Value	Unit	Source
gf	237.77	kJ/mol	Joback Method
hf	-247.82	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	76.92	kJ/mol	Joback Method
log10ws	-5.41		Aqueous Solubility Prediction Method
log10ws	-5.41		Estimated Solubility Method
logp	4.484		Crippen Method
mcvol	246.490	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
tb	802.44	K	Joback Method
tc	1035.43	K	Joback Method
tf	558.14	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.16	J/mol×K	802.44	Joback Method
cpg	886.61	J/mol×K	841.27	Joback Method
cpg	910.97	J/mol×K	880.10	Joback Method
cpg	935.65	J/mol×K	918.93	Joback Method
cpg	961.02	J/mol×K	957.76	Joback Method
cpg	987.49	J/mol×K	996.59	Joback Method

cpg	1015.46	J/mol×K	1035.43	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume