Cortol

Inchi: InChI=1S/C21H36O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2
InchiKey: FFPUNPBUZDTHJI-GBBLGXTESA-N
Formula: C21H36O5
SMILES: CC12CCC(O)CC1CCC1C2C(O)CC2(C)C1CCC2(O)C(O)CO
Mol. weight [g/mol]: 368.51
CAS: 516-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-433.12	kJ/mol	Joback Method
hf	-1038.78	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	140.86	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	1.445		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook
tb	1166.02	K	Joback Method
tc	1451.99	K	Joback Method
tf	720.19	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1343.94	J/mol×K	1166.02	Joback Method
cpg	1402.37	J/mol×K	1213.68	Joback Method
cpg	1467.38	J/mol×K	1261.34	Joback Method
cpg	1539.78	J/mol×K	1309.01	Joback Method
cpg	1620.43	J/mol×K	1356.67	Joback Method
cpg	1710.16	J/mol×K	1404.33	Joback Method
cpg	1809.81	J/mol×K	1451.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C516381&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