5«alpha»-Androstane-3«beta»,17«beta»-diol, dimethyl ether

Other names: (3«beta»,5«alpha»,17«beta»)-3,17-Dimethoxyandrostane
Inchi: InChI=1S/C21H36O2/c1-20-11-9-15(22-3)13-14(20)5-6-16-17-7-8-19(23-4)21(17,2)12-10
InchiKey: AQOCBVOXXCEOLR-UHFFFAOYSA-N
Formula: C21H36O2
SMILES: COC1CCC2(C)C(CCC3C2CCC2(C)C(OC)CCC32)C1
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	56.62	kJ/mol	Joback Method
hf	-531.69	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	5.059		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
tb	754.83	K	Joback Method
tc	982.84	K	Joback Method
tf	455.89	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.14	J/mol×K	754.83	Joback Method
cpg	962.78	J/mol×K	792.83	Joback Method
cpg	990.43	J/mol×K	830.83	Joback Method
cpg	1017.38	J/mol×K	868.83	Joback Method
cpg	1043.89	J/mol×K	906.84	Joback Method
cpg	1070.27	J/mol×K	944.84	Joback Method
cpg	1096.78	J/mol×K	982.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332980&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume