5-Cholesten-3«beta»-ol-7-one, methyl ether

Other names: (3«beta»)-3-Methoxycholest-5-en-7-one
Inchi: InChI=1S/C28H46O2/c1-18(2)8-7-9-19(3)22-10-11-23-26-24(13-15-28(22,23)5)27(4)14-1
InchiKey: YLJFYUPNPBFGPI-UHFFFAOYSA-N
Formula: C28H46O2
SMILES: COC1CCC2(C)C(=CC(=O)C3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 414.66

Physical Properties

Property code	Value	Unit	Source
gf	121.13	kJ/mol	Joback Method
hf	-625.56	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	7.222		Crippen Method
mcvol	365.080	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	4023.20		NIST Webbook
tb	968.32	K	Joback Method
tc	1200.58	K	Joback Method
tf	568.29	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.59	J/mol×K	968.32	Joback Method
cpg	1416.53	J/mol×K	1007.03	Joback Method
cpg	1448.69	J/mol×K	1045.74	Joback Method
cpg	1481.39	J/mol×K	1084.45	Joback Method
cpg	1514.93	J/mol×K	1123.16	Joback Method
cpg	1549.63	J/mol×K	1161.87	Joback Method
cpg	1585.79	J/mol×K	1200.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332985&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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