Coprostan-3-ol, methyl ether

Other names: (3«beta»,5«beta»)-3-Methoxycholestane
Inchi: InChI=1S/C28H50O/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(29-6)14-16-27(2
InchiKey: FMSSVYNONQQPON-UHFFFAOYSA-N
Formula: C28H50O
SMILES: COC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 402.70

Physical Properties

Property code	Value	Unit	Source
gf	215.68	kJ/mol	Joback Method
hf	-554.51	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	76.53	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	8.123		Crippen Method
mcvol	367.810	ml/mol	McGowan Method
pc	916.05	kPa	Joback Method
rinpol	3090.60		NIST Webbook
rinpol	3090.60		NIST Webbook
tb	891.69	K	Joback Method
tc	1111.27	K	Joback Method
tf	482.55	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1359.10	J/mol×K	891.69	Joback Method
cpg	1390.88	J/mol×K	928.29	Joback Method
cpg	1422.38	J/mol×K	964.88	Joback Method
cpg	1453.87	J/mol×K	1001.48	Joback Method
cpg	1485.65	J/mol×K	1038.08	Joback Method
cpg	1518.02	J/mol×K	1074.67	Joback Method
cpg	1551.26	J/mol×K	1111.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332887&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