Cholestan-3-ol, 4-methyl-, (3«beta»,4«alpha»,5«alpha»)-

Other names: 4-Methylcholestan-3-ol-, (3«beta»,4«alpha»,5«alpha»)-
4-«alpha»-Methyl-5-«alpha»-cholestan-3-«beta»-ol

Inchi: InChI=1S/C28H50O/c1-18(2)8-7-9-19(3)22-12-13-24-21-10-11-23-20(4)26(29)15-17-28(2

InchiKey: AMNBDMZNFAQUHN-UHFFFAOYSA-N

Formula: C28H50O

SMILES: CC(C)CCCC(C)C1CCC2C3CCC4C(C)C(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 402.70

CAS: 3903-57-9

Physical Properties

Property code	Value	Unit	Source
gf	176.15	kJ/mol	Joback Method
hf	-594.86	kJ/mol	Joback Method
hfus	40.12	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.715		Crippen Method
mcvol	367.810	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinpol	3195.00		NIST Webbook
tb	956.78	K	Joback Method
tc	1176.64	K	Joback Method
tf	516.90	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1421.94	J/mol×K	956.78	Joback Method
cpg	1453.70	J/mol×K	993.42	Joback Method
cpg	1485.75	J/mol×K	1030.07	Joback Method
cpg	1518.38	J/mol×K	1066.71	Joback Method
cpg	1551.92	J/mol×K	1103.35	Joback Method
cpg	1586.65	J/mol×K	1140.00	Joback Method

cpg	1622.89	J/mol×K	1176.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3903579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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